GeoApps in GeoDict

User Guide

GeoDict release 2022

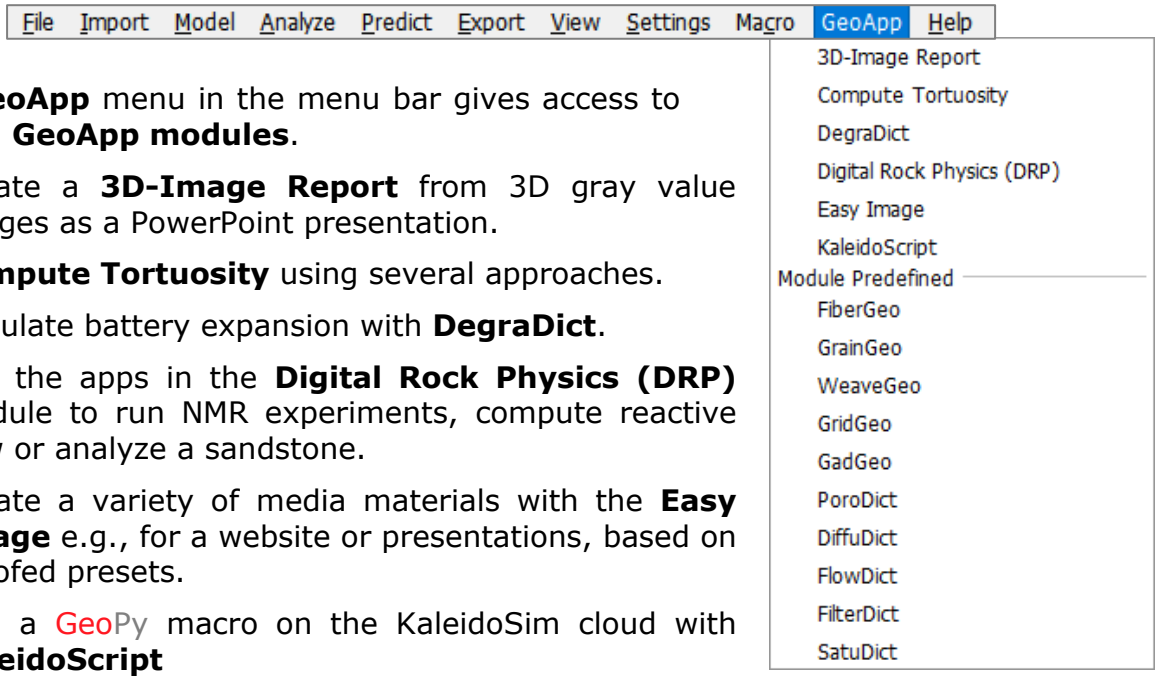
Published: March 23, 2022
Reviewed: July 18, 2022
Reviewed: September 14, 2022

GeoDict

https://doi.org/10.30423/userguide.geodict2022

GeoApps in GeoDict 2022

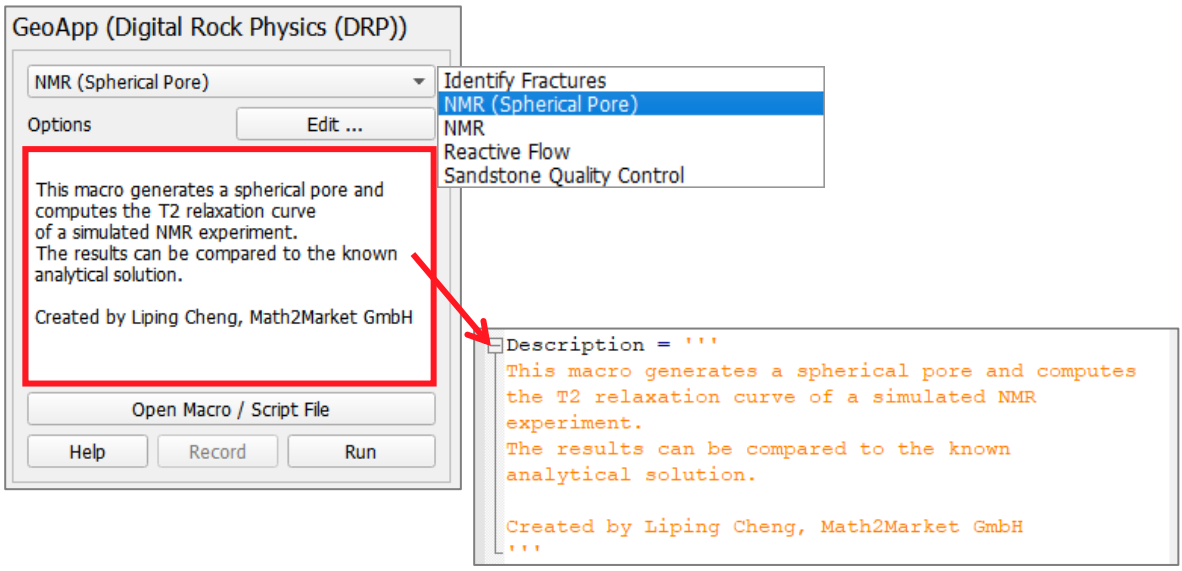
GeoDict offers great automation possibilities to enhance productivity in the form of GeoApps. All steps done by the user in GeoDict are recorded in macros. The **GeoApp** menu in GeoDict gives access to several edited macros for workflows that are often requested. Additionally, the user can add own recorded and edited parameter macros to create custom GeoApps for frequent workflows, as described on pages 35ff.



The **GeoApp** menu in the menu bar gives access to several **GeoApp modules**.

- Create a **3D-Image Report** from 3D gray value images as a PowerPoint presentation.
- **Compute Tortuosity** using several approaches.
- Simulate battery expansion with **DegraDict**.
- Use the apps in the **Digital Rock Physics (DRP)** module to run NMR experiments, compute reactive flow or analyze a sandstone.
- Create a variety of media materials with the **Easy Image** e.g., for a website or presentations, based on proofed presets.
- Run a GeoPy macro on the KaleidoSim cloud with **KaleidoScript**
- Use **Module Predefined** GeoApps for several modules, which can also be found in the corresponding module sections.

Selecting a GeoApp opens the **GeoApp** module section, located left of the Visualization area. It contains a pull-down menu listing the available GeoApps for the respective module.



GeoDict macros corresponding to the simulations are called and executed when the GeoApps are run. These macros are available in the **GeoApp** folder in the GeoDict installation folder. They can be opened with a text editor, to observe their syntax and the steps involved in the simulation. They can also be edited if the user has the privileges to change files in the GeoDict installation folder, which typically requires administrator privileges.

When selecting one of the available GeoApps, the description area displays a report about the app. In the corresponding GeoPy script, this report content can be found inside the apostrophes after **Description = ''' '''** and can be edited at any time after opening the script with a text editor. For the **NMR (Spherical Pore).py** app from the GeoApp module **Digital Rock Physics**, the text in the macro and the description area is shown above.

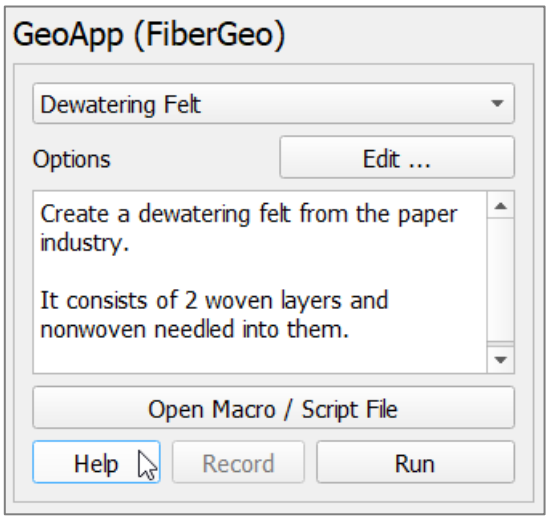
Click the **Options' Edit ...** button to edit the parameters of the macro.

By clicking **Open Macro / Script File**, the macro file containing all steps for the app simulations can be accessed in a text editor. For detailed information about GeoPy and editing GeoDict macros refer to the Automation & Scripting handbook of this User Guide.

Clicking **Run** runs the app.

Module Predefined macros are also contained in the respective modules and described in the corresponding User Guide handbooks.

Open the corresponding handbook by clicking **Help** in the GeoApp module section. In the example on the right, the **Help** button opens the FiberGeo handbook.

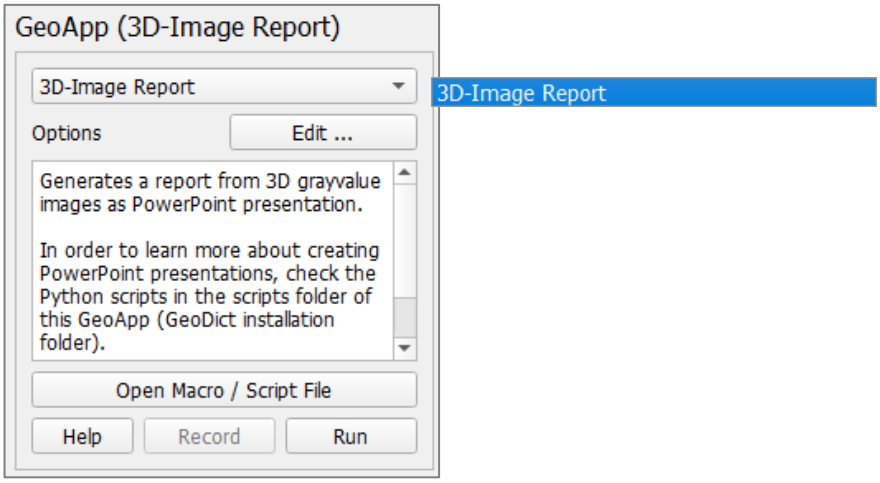


THE GEOAPPS SHIPPED WITH GEODICT

The GeoApps delivered with GeoDict are described shortly in the following. Please ask support@math2market.de if you want to know more details about the specific parameters used in theses apps and the functionality they provide.

3D IMAGE REPORT

The **3D-Image Report** app generates a report from 3D gray value images as a PowerPoint presentation.

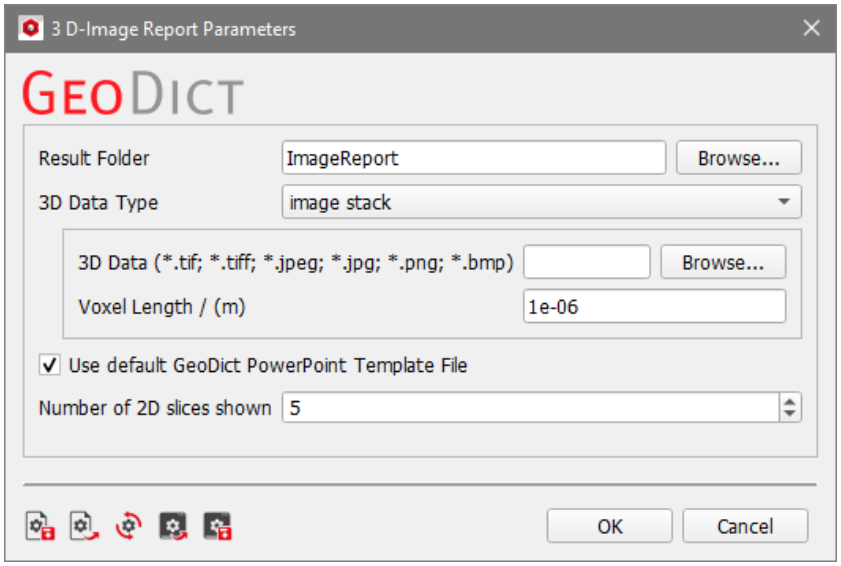


In order to learn more about creating PowerPoint presentations, refer to the Automation & Scripting handbook of this User Guide or check the Python scripts in the scripts folder of this GeoApp (GeoDict installation folder).

Modules needed to run this GeoApp: ImportGeo-Vol

Clicking **Edit** opens the **3D-Image Report Parameters** dialog.

The input parameters include **Result Folder**, **3D Data Type**, **Voxel Length**, **Use default GeoDict PowerPoint Template File**, and **Number of 2D slices shown**.

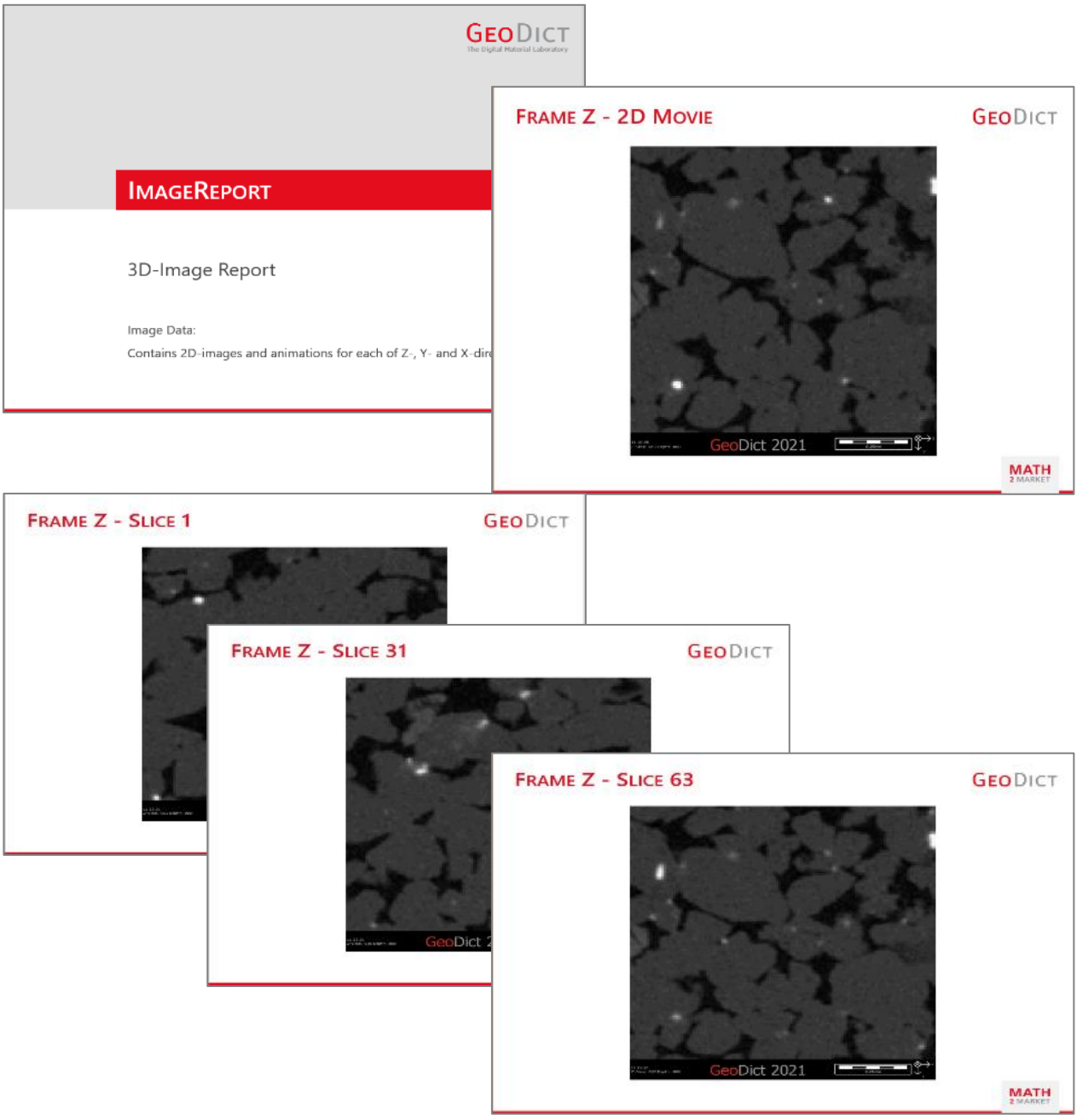


The detailed explanations of the parameters and how to customize the PowerPoint Template File are found in the GeoApp for 3D-Image PowerPoint reports tutorial. Also, helpful tooltips appear, when hovering the cursor over the parameters.

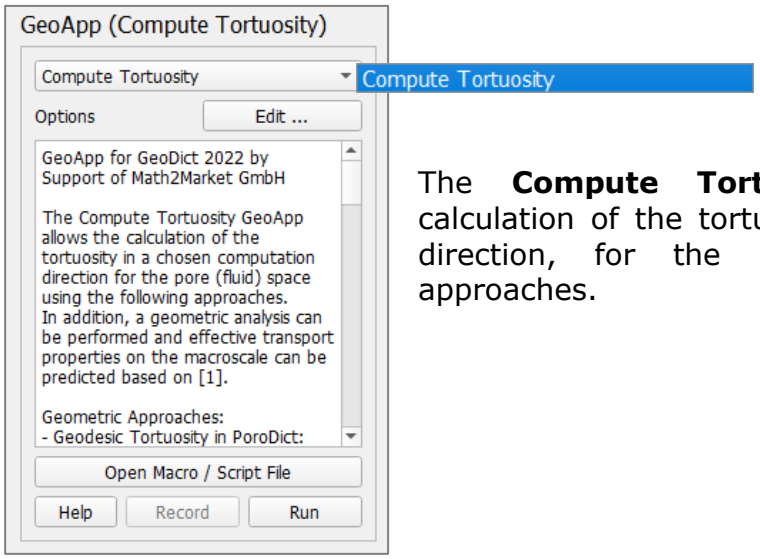
The parameters can be modified if needed. Otherwise, click **OK** to close the dialog, go back to the **GeoApp** section and click **Run**.

The PowerPoint report is found in the result folder after the GeoApp run is finished.

The presentation contains a title slide and, for each of the Z-, Y-, and X-Directions, the set amount of 2D image slices is included. Three 2D videos can be started by clicking the corresponding slide. The videos show the whole image data from this axis. A careful examination of the PowerPoint presentation slides, running as a loop, may reveal previously unknown image artifacts.



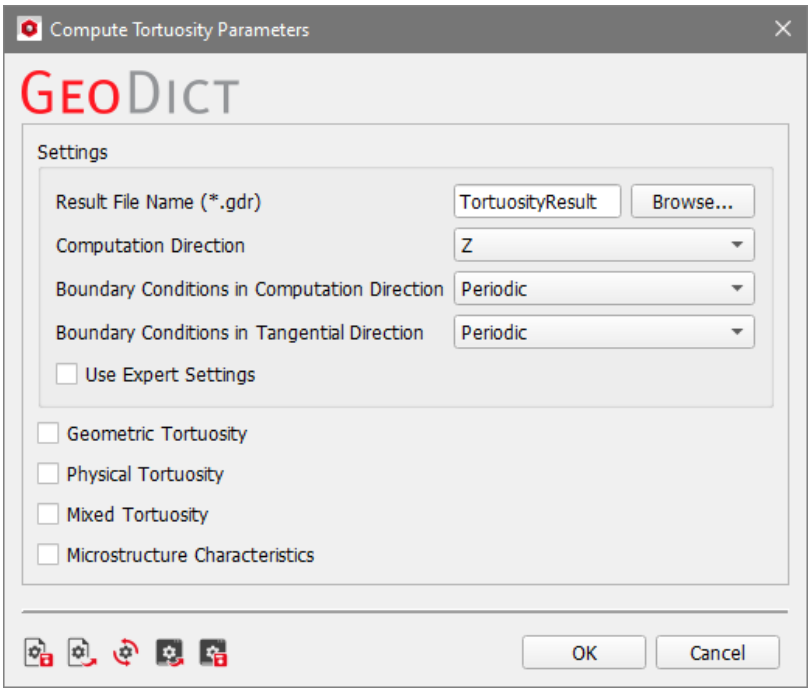
COMPUTE TORTUOSITY



The **Compute Tortuosity** GeoApp allows the calculation of the tortuosity in a chosen computation direction, for the pore space, using different approaches.

Modules needed to run this GeoApp (depending on the selected options): PoroDict, MatDict, DiffuDict, ConductoDict, FlowDict, AddiDict

In addition, with the **Compute Tortuosity** app, a geometric analysis can be performed and effective transport properties on the macroscale can be predicted based on [1]. Generally, three different kinds of tortuosities can be computed: geometric tortuosities, which are directly derived from the microstructure, physics-based tortuosity, which are indirectly derived by transport mechanisms, and mixed tortuosities, which use a mixture determination from geometric analysis and physical transportation phenomena. Clicking **Edit** opens the **Compute Tortuosity Parameters** dialog.



Select a **Result File Name** and the **Computation Direction** in the **Settings** panel. Also, the **Computation Direction** and **Boundary Conditions** can be changed.

Then choose which properties should be computed.

Two options are available for **Geometric Tortuosity**. These tortuosities are directly derived from the morphological characteristics of the analyzed structure and are well-defined by the structure only.

The general definition of the Geometric tortuosity is the comparison of the effective geometric pathlength L_{eff} to the shortest geometric pathlength L_0:

$$\tau = \frac{L_{eff}}{L_0}$$

The geometric tortuosities available are:

- **Geodesic Tortuosity** in PoroDict: Computing the mean geodesic tortuosity from the percolation pathway starting from every voxel in the inlet. I.e., the shortest path in pore space is compared to the direct path.
- **Percolation Tortuosity** in PoroDict: Computing the mean value of the percolation pathways with the 50 largest diameters. I.e., the length of the path of large particles (largest possible diameters) through the structure (median axis) is compared to the direct path.

Four options are available for **Physical Tortuosity**. These tortuosities are indirectly derived. The physics-based tortuosities do not use the geometric pathlengths

$$\tau \neq \frac{L_{eff}}{L_0}$$

Physical tortuosities are determined using effective properties to deduce a tortuosity value indirectly. Therefore, microstructure effects as bottleneck-effects are included. A physical tortuosity is only meaningful if it bases on a transport phenomenon that is relevant to the simulated material. Thus, different tortuosities can be determined depending on the dominating transport mechanism: diffusion of molecules or ions, conductivity of electrons etc. For an example consider the effective diffusion of gas through a porous membrane in comparison to the self-diffusion of the gas. Then, the diffusion tortuosity is of interest [2]. GeoDict can output both, the value for the **tortuosity** τ and the value of the **tortuosity factor** κ by comparing the effective diffusion to self-diffusion:

$$\tau_{\mathrm{indir,diff}} = \sqrt{\kappa_{\mathrm{indir,diff}}} = \sqrt{\frac{\varepsilon}{\mathrm{D_{rel}}}}$$

where ε is the porosity and D_{rel} the relative diffusivity due to the porous-media dependent part of the effective diffusion. GeoDict can output both, the value for the tortuosity τ and the value of the tortuosity factor κ. These numbers can be converted in each other by the general relation between τ and κ:

$$\tau = \sqrt{\kappa}$$

The available physical tortuosities are:

- **Diffusion Tortuosity** in DiffuDict: Diffusion as indirect, physical approach [3]. The tortuosity will be extracted from the DiffuDict **Laplace** and **Knudsen** Diffusion result files (GDR), respectively.
- **Conduction Tortuosity** in ConductoDict: **Electrical** and **Thermal** conductivity as indirect, physical approach [4]. The tortuosity will be extracted from the respective ConductoDict result file (GDR).

Four options are available for **Mixed Tortuosity.** The mixed tortuosities are derived from a mixed determination including the geometrical analysis of streamlines and pathways from simulations of diffusion, flow, advection, etc. The available mixed tortuosities are:

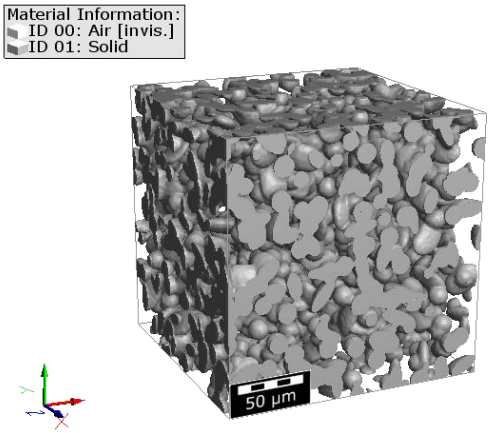
- **Tortuosity from Laplace Diffusion Flux** in DiffuDict [5]: The mean value of DiffuDict Laplace diffusion flux streamlines and/or the tortuosity is calculated based on the volume average of DiffuDict Laplace diffusion flux
- **Tortuosity from Stokes Flow Velocity** in FlowDict [6]: The mean value of the streamline length of FlowDict Stokes flow velocity streamlines and/or the tortuosity is calculated based on the volume average of FlowDict Stokes flow velocity.
- **Tortuosity from Particle Advection** in AddiDict: Computing the mean value of the particle path length for advection.
- **Tortuosity from Particle Diffusion Path Length** in AddiDict: The mean value is calculated based on effective isotropic diffusivity

Additionally, to the different tortuosities, the **Compute Tortuosity** GeoApp can calculate **Microstructure Characteristics**. Three options are available:

- **Characteristic Diameters** from **Granulometry** or **Porosimetry** in PoroDict: Computing D10, D50, and D90.
- **Surface Area** in MatDict: Specific surface area between pore space and solid materials.

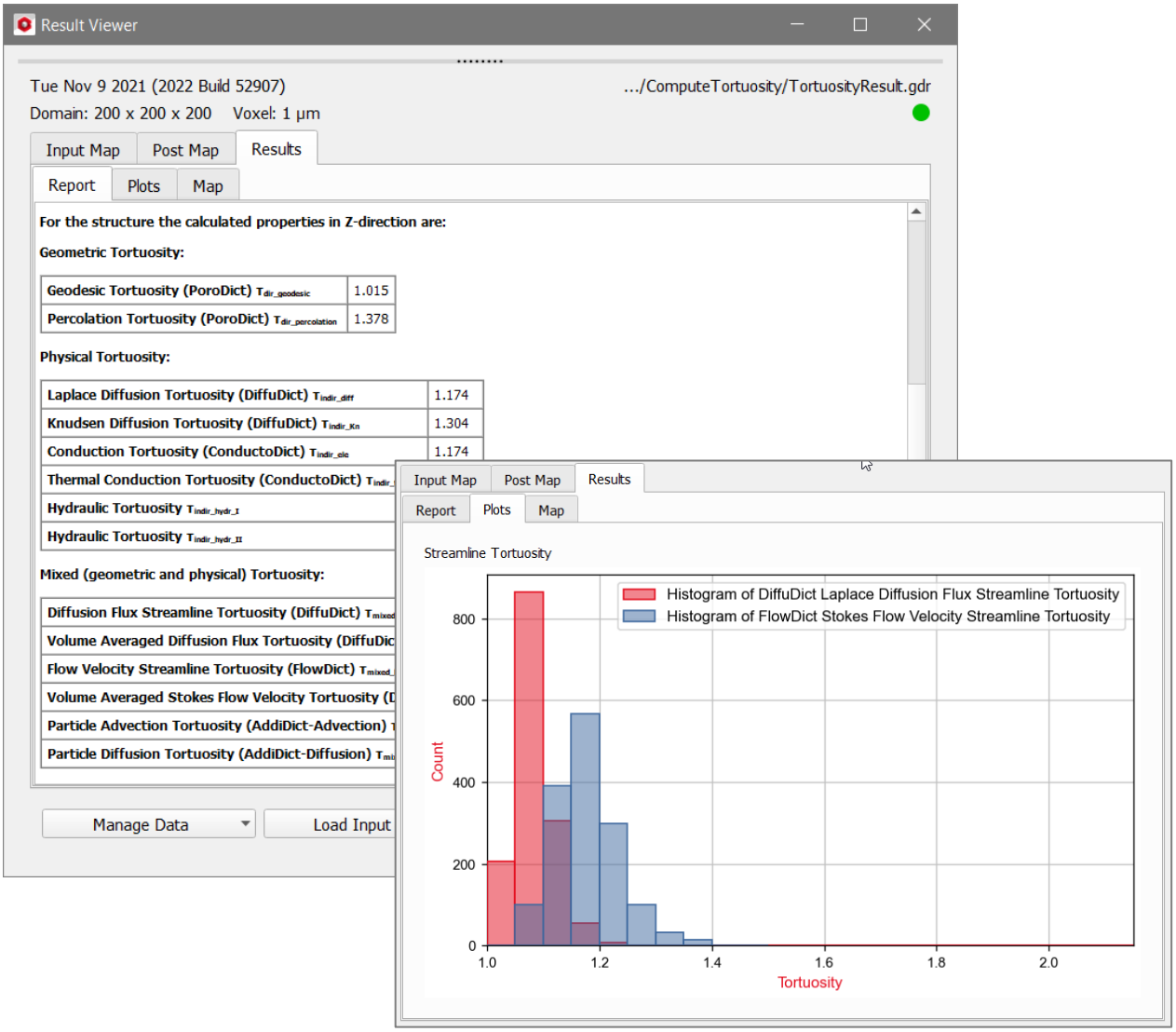
After the **Compute Tortuosity** app has finished, the Result Viewer of the result file opens.

The result file provides detailed information about the formulas used to calculate the different tortuosities, the microstructure characteristics, the pore phase and transport properties, as well as those used to predict effective transport properties.

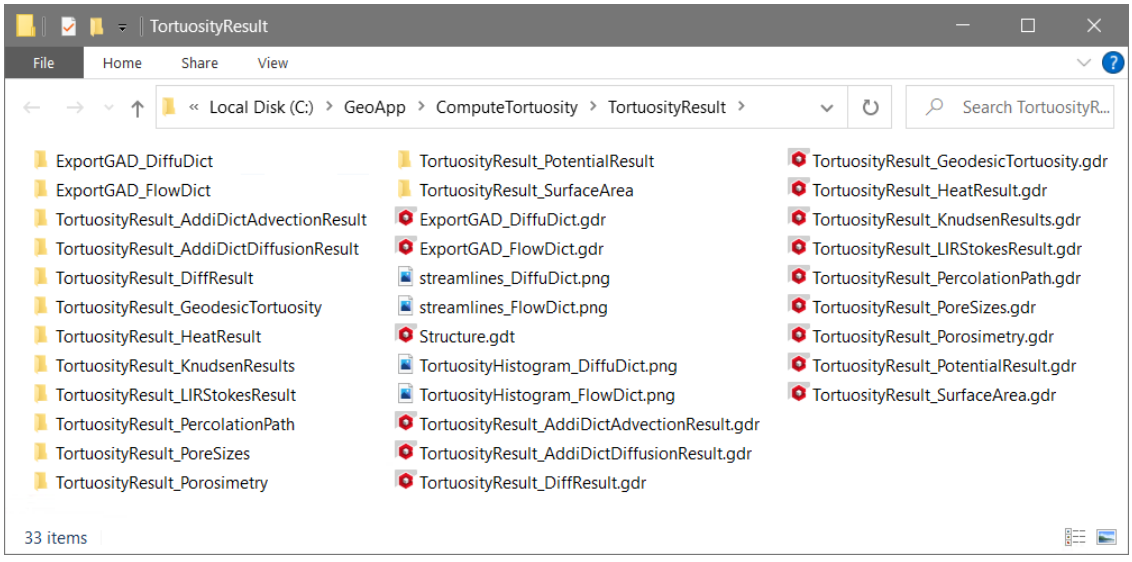


Depending on the selection in the **Compute Tortuosity Parameters** dialog, the results are given in tables.

If the calculation of the tortuosity based on streamlines was selected, the evaluation of streamline length is shown as a **Streamline Tortuosity** plot.



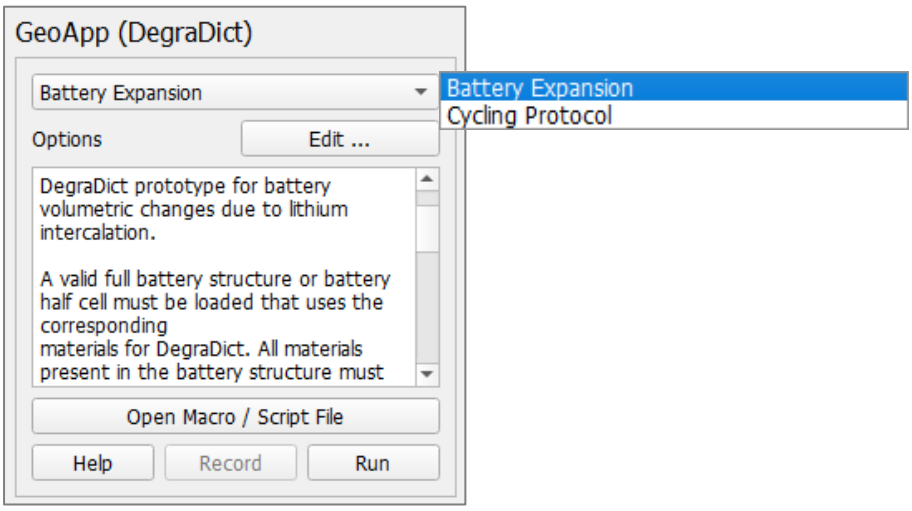
Additionally, the corresponding result folder contains the detailed GeoDict results corresponding to the respective simulations.



DEGRADICT

The **DegraDict** GeoApp contains the following apps, selectable from the pull-down menu:

- **Battery Expansion:** simulate one-way battery volumetric changes due to lithium intercalation.
- **Cycling Protocol:** simulate battery cycling, taking into account its volumetric changes of the structure during charging and discharging.



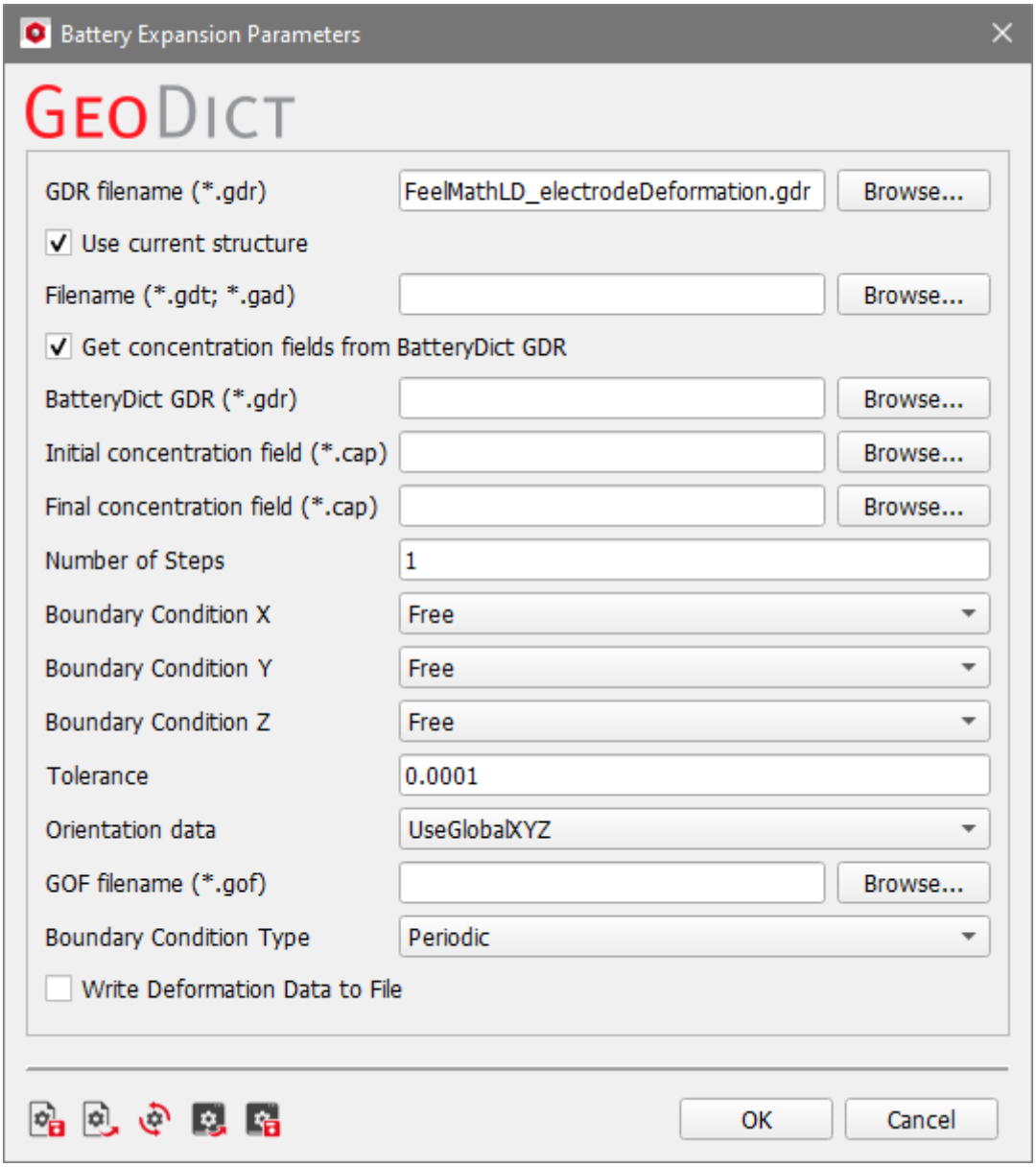
A special **DegraDict** license is required to use this prototype. Please contact electrochemistry@math2market.de for further information.

Battery Expansion

The **Battery Expansion** app is a **DegraDict** prototype for one-way battery volumetric changes due to lithium intercalation. The app uses ElastoDict's FeelMath solver to run a deformation simulation based on the concentration fields from a preliminary successfully finished battery charge or discharge analysis.

Modules needed to run this GeoApp:
BatteryDict, ElastoDict

Clicking **Edit...** opens the **Battery Expansion Parameters** dialog. The parameters refer to FeelMath-LD settings and can be modified if needed (for details, see tooltips and ElastoDict User Guide). Otherwise, select corresponding **BatteryDict GDR** and click **OK** to close the dialog, go back to **GeoApp** section, and click **Run**.



A valid structure must be loaded. A valid structure is either a full battery structure created, for example, with the **Design Battery** module in BatteryDict or a half-cell, i.e. an anode or cathode consisting of materials allowed in **DegraDict**. All materials

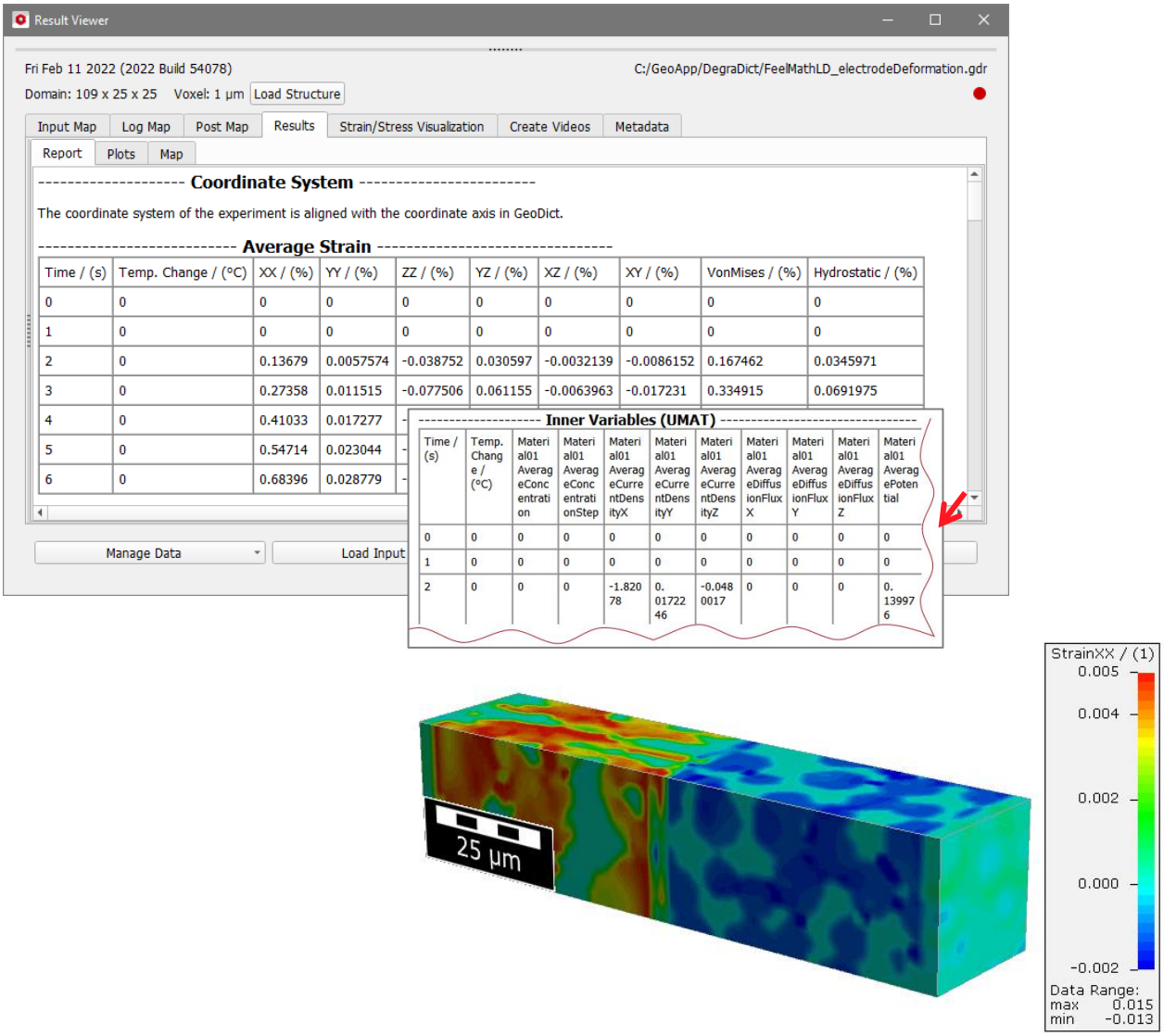
present in the battery structure must use the **Lithium Intercalation UMAT**. Predefined materials available in the GeoDict Material Database are:

- Copper as Anode Current Collector,
- Graphite as Anode Active Materials,
- PVDF Binder + Carbon Black as Binder for Anode and Cathode,
- Polypropylene as Separator,
- NMC333 as Cathode Active Material,
- Aluminum as Cathode Current Collector.

All used non-fluid materials must be set as **Solid** for the BatteryDict simulation. Currently no porous materials can be used for DegraDict computations.

Use the volume fields (concentration fields CAPs) from a BatteryDict Charge simulation of the same size as the loaded or current structure.

When the simulation finishes, the result file is written and can be opened manually by choosing in the menu bar **File → Open Results (*.gdr)...** . The **Result Viewer** shows the deformation results in the **Results → Report** tab. Additionally to usual ElastoDict outputs of average stresses and strains (caused by lithium concentration fields in the case), **Inner Variables (UMAT)** are available, e.g., concentrations, densities, diffusion fluxes, potentials. In the following example, see the anode expansion at the left part of a battery after its charging.



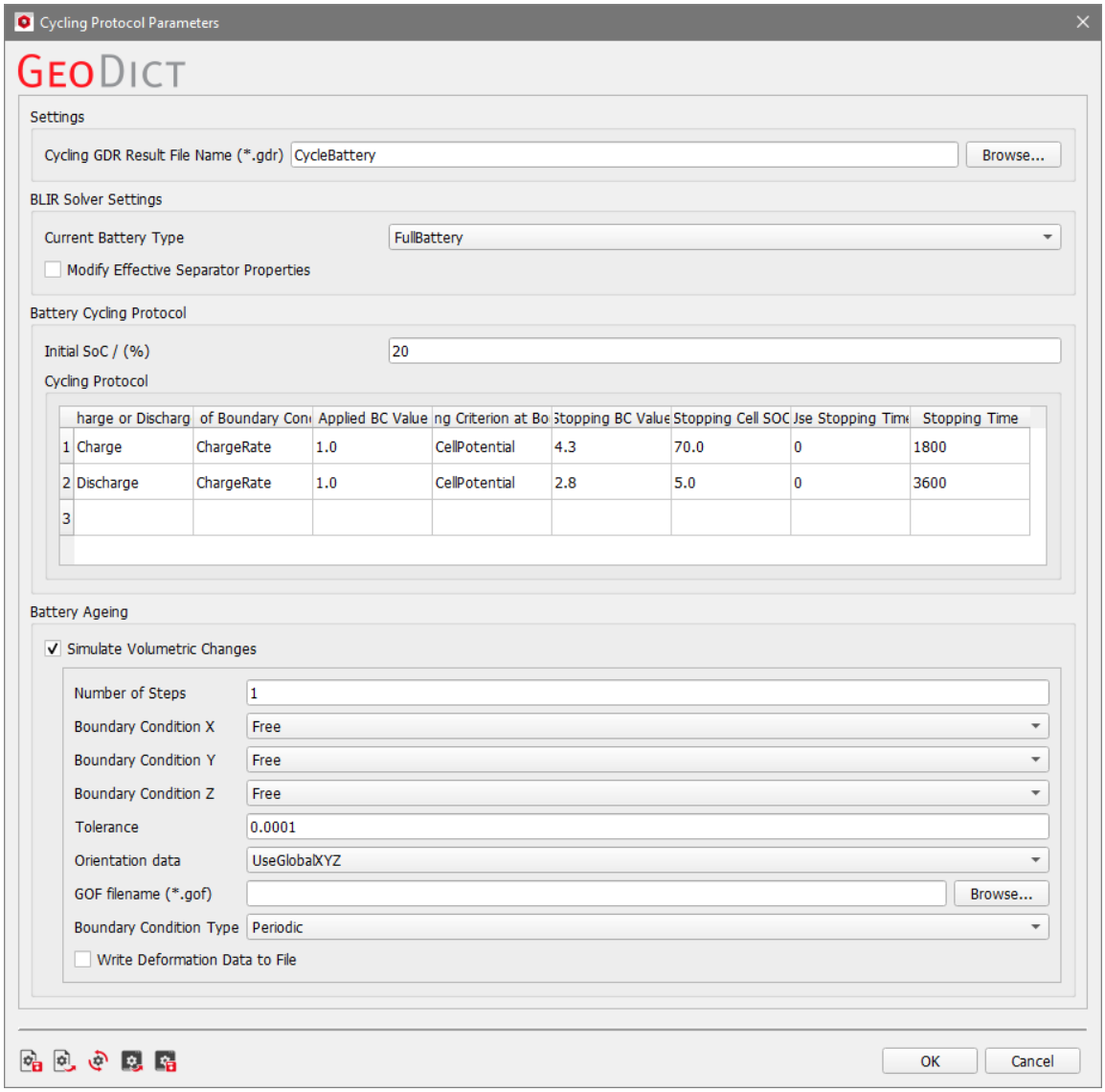
CYCLING PROTOCOL

The **Cycling Protocol** app is a **DegraDict** prototype for battery cycling, including volumetric changes due to lithium intercalation. The app runs a user predefined cycling profile where stages of charging and discharging alternate with successive battery deformations according to Battery Expansion Protocol.

Modules needed to run this GeoApp:
BatteryDict, ElastoDict

Clicking **Edit...** opens the **Cycling Protocol Parameters** dialog. The parameters can be modified if needed. Tooltips describe all those options in more detail.

Otherwise, click **OK** to close the dialog and go back to **GeoApp** section.



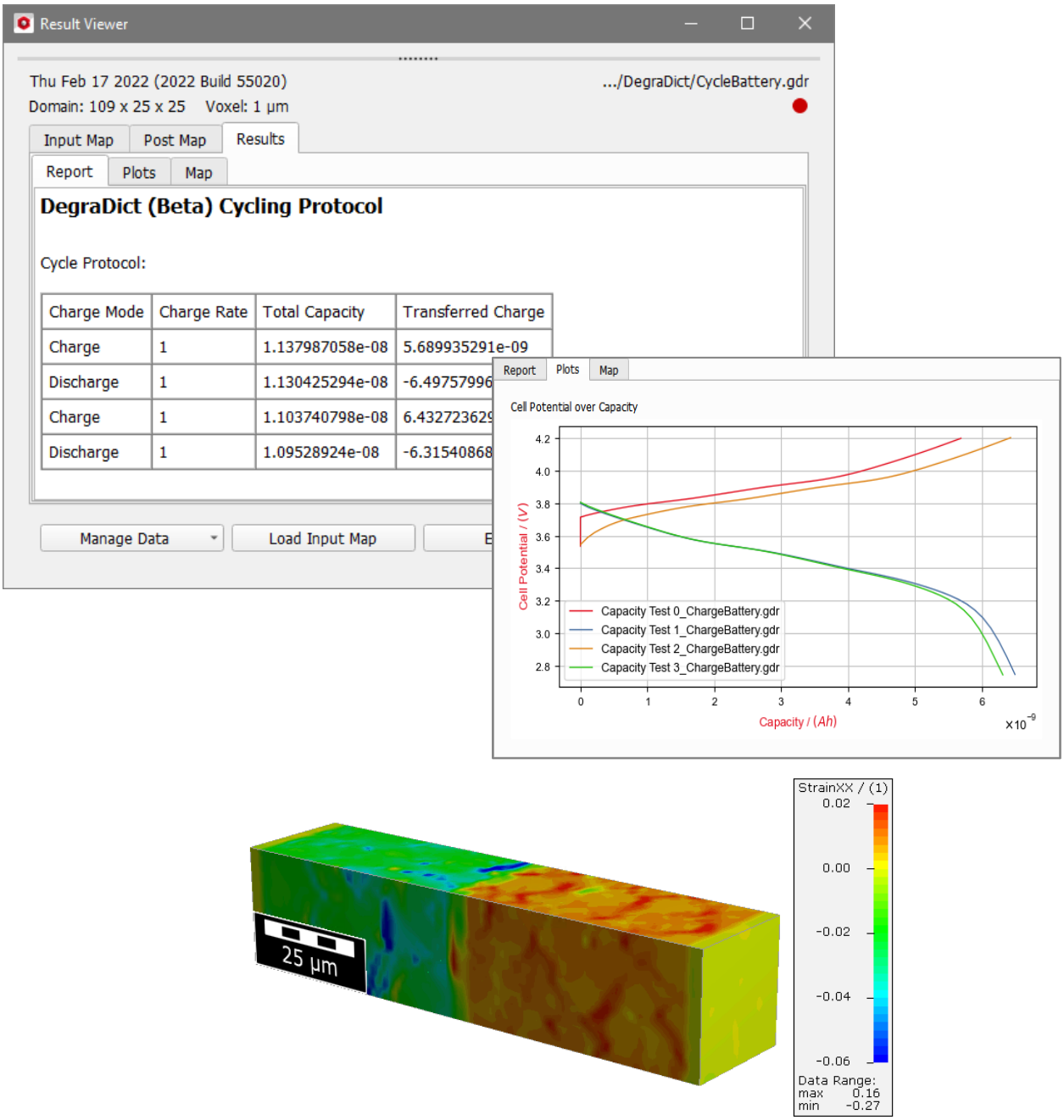
Before click **Run**, load a valid battery structure as it is described in the previous section on page 10ff, select its **Current Battery Type** and additionally check to use corresponding Electrical Conductivity Laws:

- for current collectors – **Current Collector**,
- for the separator – **Separator**.

Define a charging profile in the parameter section **Battery Cycling Protocol** (for details, see BatteryDict User Guide).

In the parameter section of **Battery Ageing**, **Simulate Volumetric Changes** must be checked to activate and set variables of Battery Expansion Protocol. After each step of the charging profile, the battery structure will be deformed according to the changes in lithium concentration from the initial time step to the final time step.

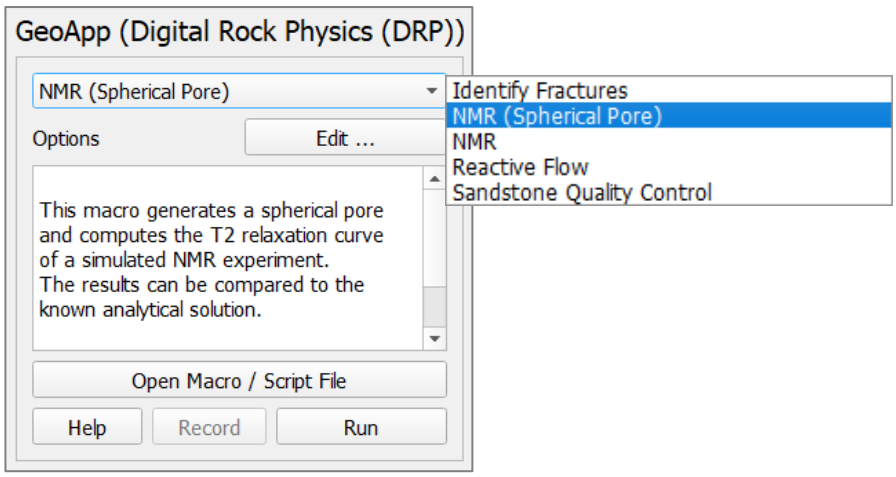
When the cycling simulation finishes, the **Result Viewer** opens the result file (*.gdr) automatically. The cycling results are shown as a table in the **Results → Report** tab and can be found as a plot in the tab **Results → Plots**. The mechanical simulation results computed after each step of cycling profile and described on page 11, can be open manually in the menu bar **File → Open Results (*.gdr)...** and by selecting corresponding **#X_ChargeBattery_FeelMath.gdr** from the result folder. In the next example, see the cathode expansion at the right part of a battery due to discharging step.



Digital Rock Physics (DRP)

The **Digital Rock Physics (DRP)** GeoApp contains the following apps, selectable from the pull-down menu:

- **Identify Fractures**: analyze the pore morphology and segment the chosen material into fractures, small and large pores.
- **NMR (Spherical Pore):** run an NMR experiment on a spherical pore.
- **NMR:** run an NMR experiment on the current structure.
- **Reactive Flow:** compute reactive flow for the current structure.
- **Sandstone Quality Control**: run a quality control on the current structure.



Identify Fractures

The **Identify Fractures** app analyzes the pore morphology and segments the chosen Material ID into fractures, small and large pores. The macro applies multiple runs of **Identify Pores** and the corresponding **Identify Pores Post Processing** to distinguish between pores and fracture phase.

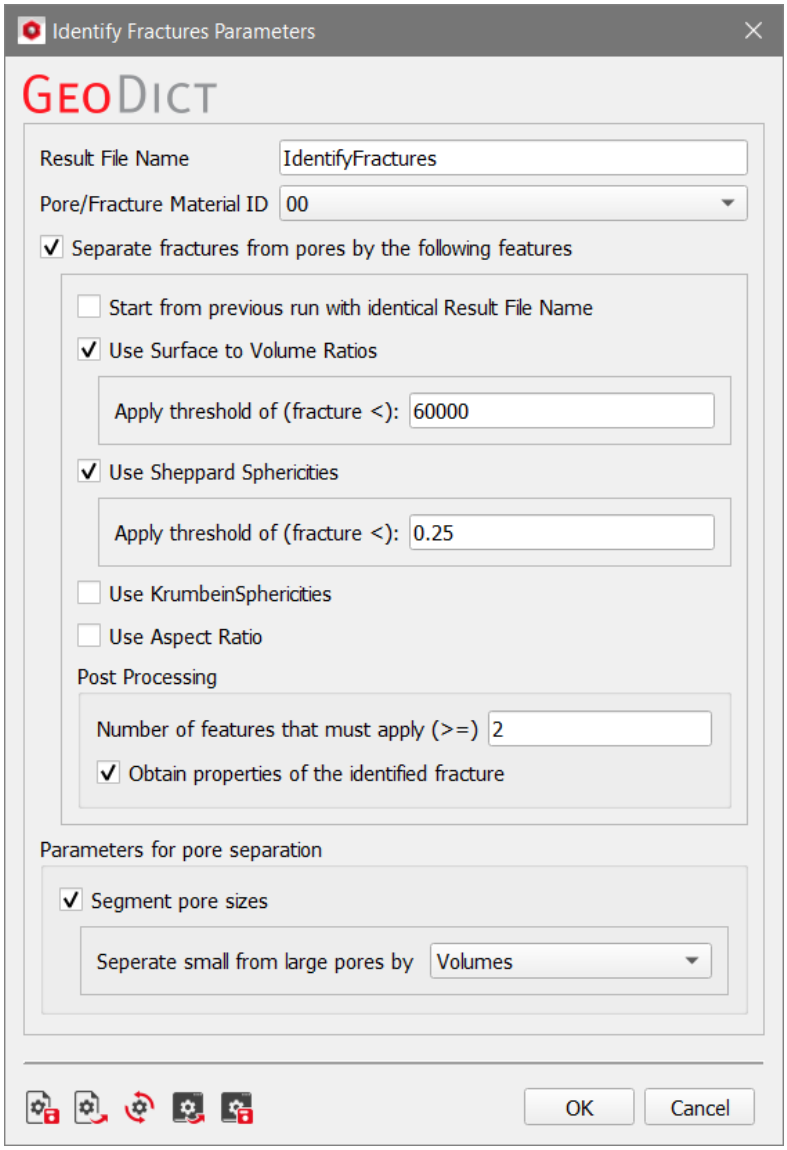
Modules needed to run this GeoApp: PoroDict

Clicking **Edit...** opens the **Identify Fractures Parameters** dialog.

There are two main features of the **Identify Fractures** app.

The first main feature **Separate fractures from pores by the following features** segments the selected **Pore/Fracture Material ID** into fracture and pore phase.

The second main feature **Segment pore sizes** allows the differentiation between small and large pores. When both features are activated, the differentiation of the pore sizes will be performed only on the pore phase, not on the fracture phase.



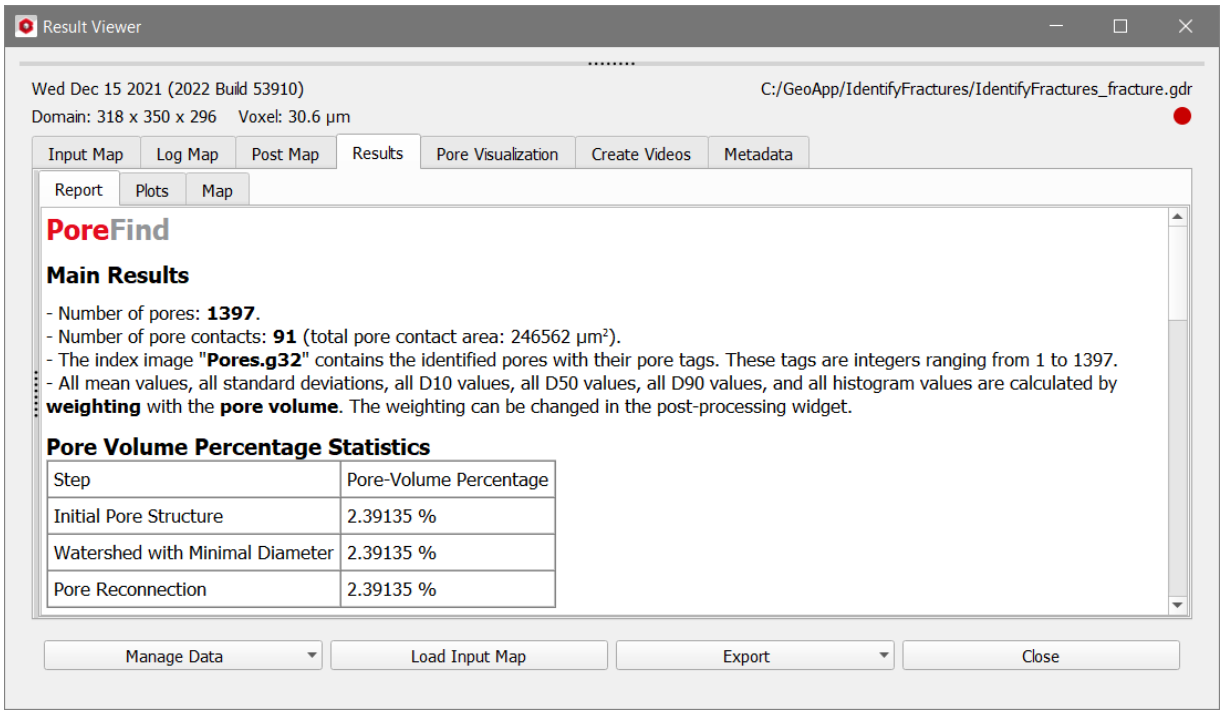
For the fracture identification, the chosen threshold values consider void space in a structure as a fracture if the values are below a chosen threshold for each parameter. The parameters can be modified if needed. The default threshold values may already segment fractures correctly. To improve the result, adjust the threshold values accordingly to the current structure. In the **Post Processing** section, the **Number of features that must apply** to identify a fracture phase can be chosen. The number must always be smaller or equal to the number of activated features. When **Obtain properties of the identified fracture** is activated, an additional instance of **Identify Pores** is executed on the previously identified fractures.

If **Identify Fractures** was executed on a structure but the segmentation needs to be improved, the app should be re-executed to obtain the best result iteratively. That can be done by re-executing the app with different values until a sufficient result is achieved. To save time, activate **Start from previous run with identical Result File Name**. This skips the first **Identify Pores** instance and uses the previous created *.gdr to execute **Post Processing**.

Click **OK** to close the dialog, go back to the **GeoApp** section, and click **Run**.

When the macro run is finished, and the checkbox of **Obtain properties of the identified fracture** is checked, the **Result Viewer** of the result file (*.gdr) opens automatically. Find the results in the **Results** → **Report**, **Results** → **Plots** and **Pore**

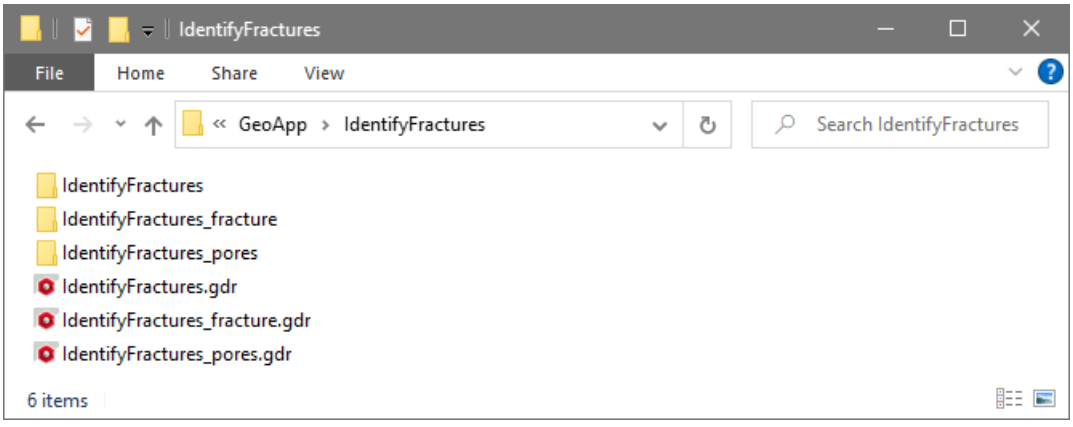
Visualization tabs. The result file is created with **PoroDict → Identify Pores**. Thus, for detailed information about the result file content refer to the PoroDict User Guide.



Three result files and result folders are generated and can be found in the project folder.

The prefix is based on the chosen Result File Name (default is **IdentifyFractures**). The **IdentifyFractures** folder contains the results of the **Identify Pores** instance which was executed on the structure. The thresholding of the fractures by features, which can be performed with the script, is executed on the contained **IdentifyFractures.gdr**. When **Obtain properties of the identified fracture** is activated, the **IdentifyFractures_fracture** folder contains results of the respective **Identify Pores** run. When **Segment pore sizes** is activated, the pores in the structure are segmented by their **Volume** or **Equivalent diameters**.

In this case, the folder **IdentifyFractures_pores** is created which contains the **Identify Pores** run performed on the pores.



NMR (Spherical Pore)

The **NMR (Spherical Pore)** app generates a spherical pore and computes the T2 relaxation curve of a simulated NMR experiment. The results can be compared to the known analytical solution.

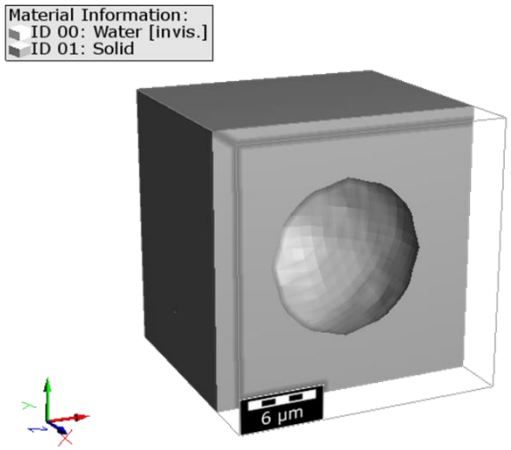
Modules needed to run this GeoApp: AddiDict

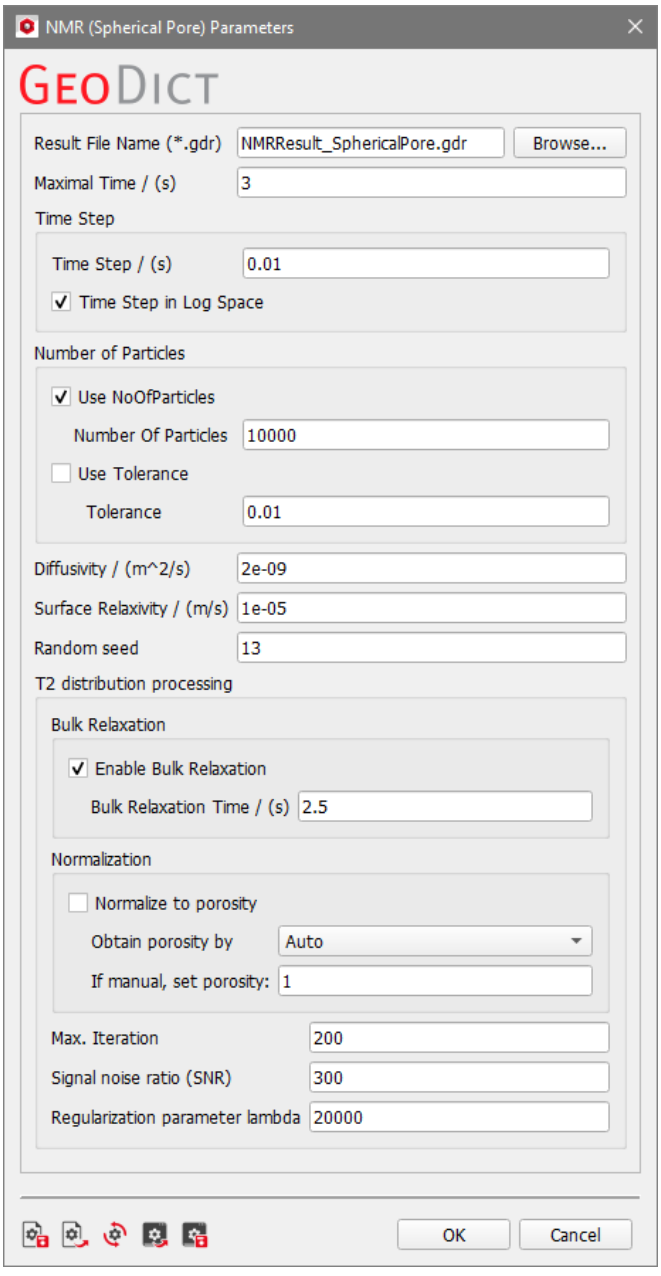
Clicking **Edit...** opens the **NMR (Spherical Pore) Parameters** dialog. The input parameters include **Result File Name**, **Maximal Time**, **Time Step**, **Number of Particles**, **Diffusivity**, **Surface Relaxivity**, **Random seed**, **Bulk Relaxation**, and **Normalization**.

Tooltips describe the parameter options and detailed explanations of the parameters are found in the tutorial Random-walk method to simulate T2 of NMR.

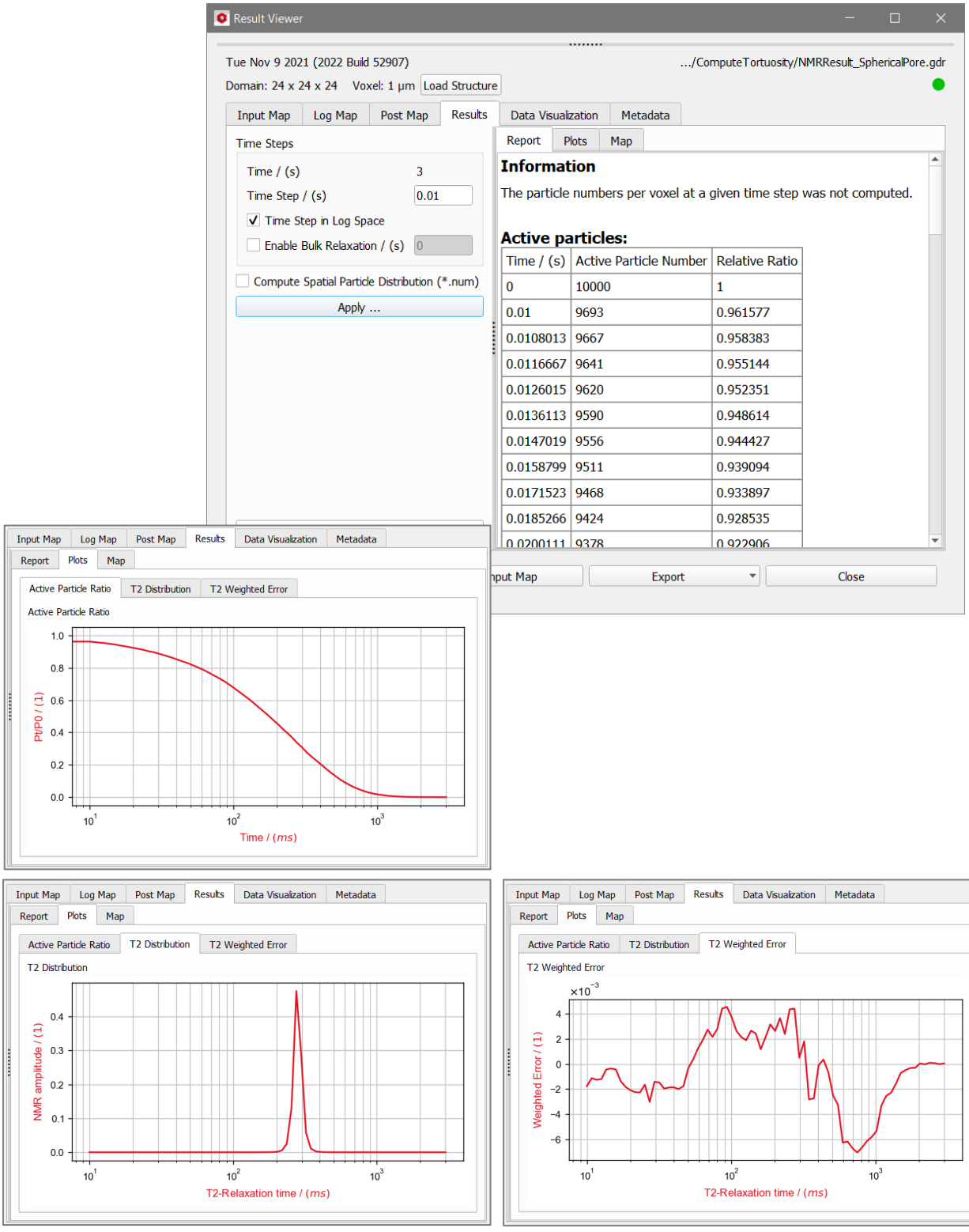
The parameters can be modified if needed. Otherwise, click **OK** to close the dialog, go back to **GeoApp** section, and click **Run**.

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically, and in the Visualization area a hollow cube with a spherical pore is shown; here clipped in Z-direction.





The **Results** → **Report** tab (*below*) of the **Result Viewer** shows the table for the number of **Active particles** and the resulting relative ratio vs. the simulation time. In the **Results** → **Plots** tab (*below-right*), the plot of **Active Particle Ratio**, corresponding to the values of the Active particles table, the plot of **T2 Distribution**, and **T2 Weighted Error** are shown. For more details on the results, refer to the NMR tutorial.



NMR

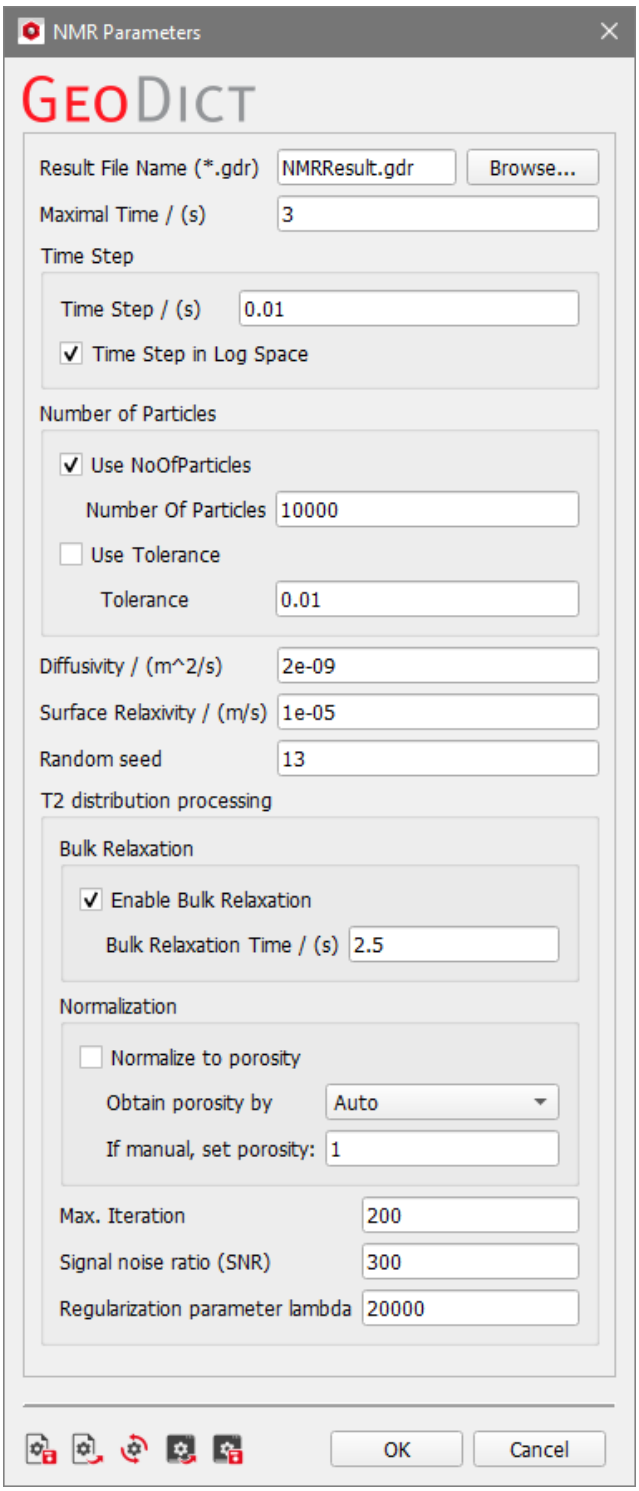
The **NMR** app computes the T2 relaxation curve of a simulated NMR experiment on the current 3D structure. Thus, it is used for general NMR simulation purposes, while the **NMR (Spherical Pore)** app creates a close pore structure and simulates on it.

Modules needed to run this GeoApp: AddiDict

After loading a 3D structure, clicking **Edit** for the **NMR** app opens the **NMR Parameters** dialog. The predefined parameters are the same as those for the **NMR (Spherical Pore)** app. Modify them according to the desired NMR expriment and start the simulation.

Tooltips describe the parameter options.

Two NMR simulation examples, one for a Bentheim sandstone and the other for an Obernkirchen sandstone, are found in the NMR tutorial.



Reactive Flow

The **Reactive Flow** app computes dissolution and precipitation of mineral phases during continuous inflow of reactants (e.g., acid) and predicts:

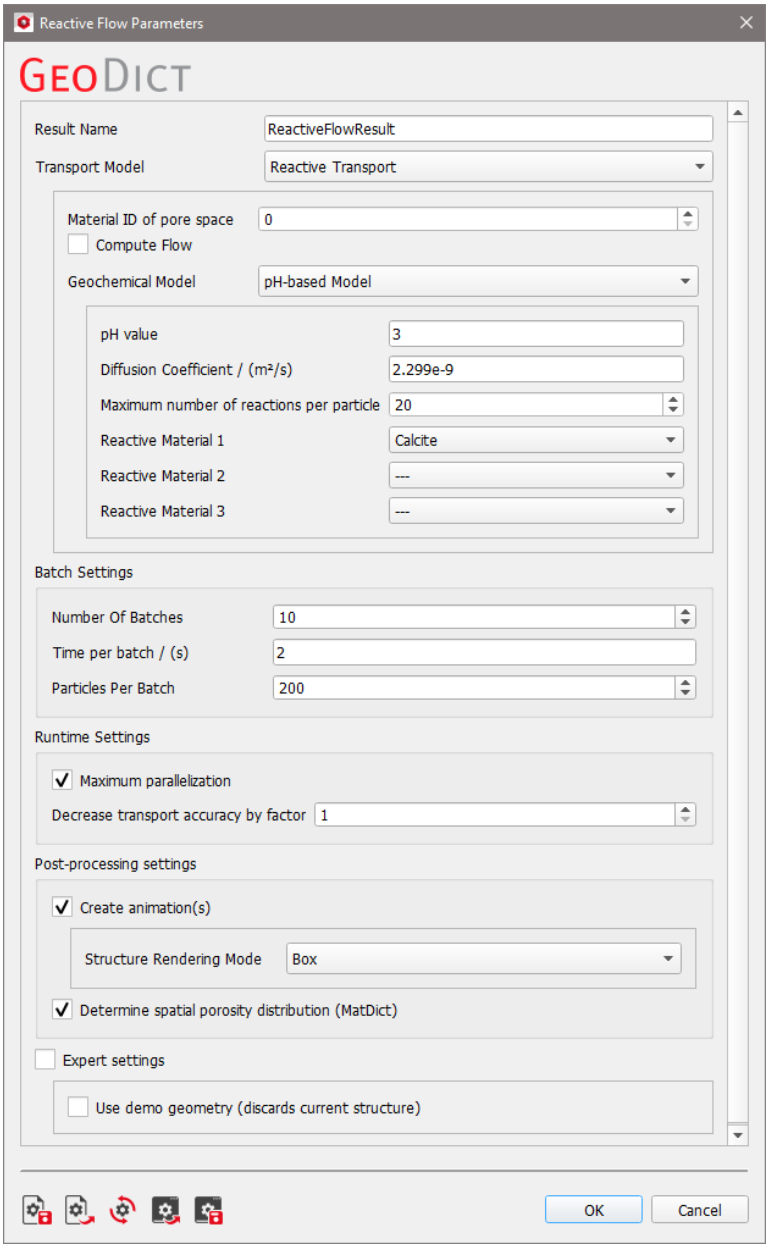
- Permeability reduction & enhancement (porosity-permeability relationship)
- 4D rock alteration: automated generation of animations that enable visual determination of the precipitation and dissolution patterns in addition to the analysis via various plots that are generated automatically.
- Chemical transport in the geometry, determined on the voxel scale

Modules needed to run this GeoApp: AddiDict, optionally: FlowDict, PoroDict

Clicking **Edit** opens the **Reactive Flow Parameters** dialog.

Choose a **Result Name** for the resulting GeoDict result file (*.gdr) and the corresponding result folder.

Tooltips describe the parameter options in more detail.



This GeoApp is applicable to many different research and business topics such as "Acidizing treatments in carbonate reservoirs", "CO_2 sequestration", "Nuclear Waste Storage", "Environmental Remediation", and "Hydrogen Underground Storage".

Therefore, two **Transport Models** are available in the GeoApp:

- **Reactive Flow**, one-directional, with or without an injection velocity
- **Reactive Counter-Diffusion** based on typical lab experiment setups

For solving **Reactive Flow** for the various application areas, the geochemical calculator PhreeqC (USGS) is coupled to GeoDict to offer four different **Geochemical Models** in GeoDict based on the Lagrangian Transport method:

- **PhreeqC Geochemical Equilibrium Thermodynamics**: Simulate Equilibrium Reactions with PhreeqC applying user-defined complex fluid compositions at ambient or reservoir conditions to dissolve and/or precipitate selected reactive mineral phases
- **PhreeqC Calcite Reaction Kinetics**: Simulate kinetically-controlled Calcite Dissolution and/or Precipitation with individual fluid compositions at ambient conditions applying the kinetics of [7] given in the PhreeqC default database *phreeqc.dat*
- **Reaction Rate Model**: Kinetic dissolution/precipitation based on a priori known user-defined and mineral-specific reaction rates at particle-rock collisions
- **pH-based Model**: Mineral dissolution due to acid injection, reactivity is controlled by pH value and particle-rock collisions based on the approach of [8], see also our dedicated technical report [12]

The parameters can be modified if needed. Otherwise, click **OK** to close the dialog, go back to **GeoApp** section and click **Run**.

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically. The results show Number of Batches, Total Simulation Time, Total Reaction Time, and Delta Porosity in the **Results** → **Report** tab.

Four plots are found under the **Results** → **Plots** tab: Porosity, Porosity gradient, Reaction rate, and Damkoehler number.

In the following, see some sample visualizations:

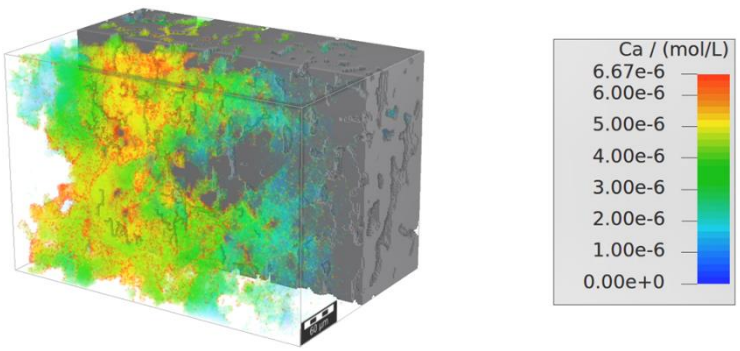


Figure 1.

Digital Reactive Flow Experiment considering the entire aqueous geochemistry here showing an intermediate result of a digital kinetically-controlled acidizing treatment of a Grosmont carbonate rock ([9]) upon inflow of a hydrochloric acid at pH 5.5

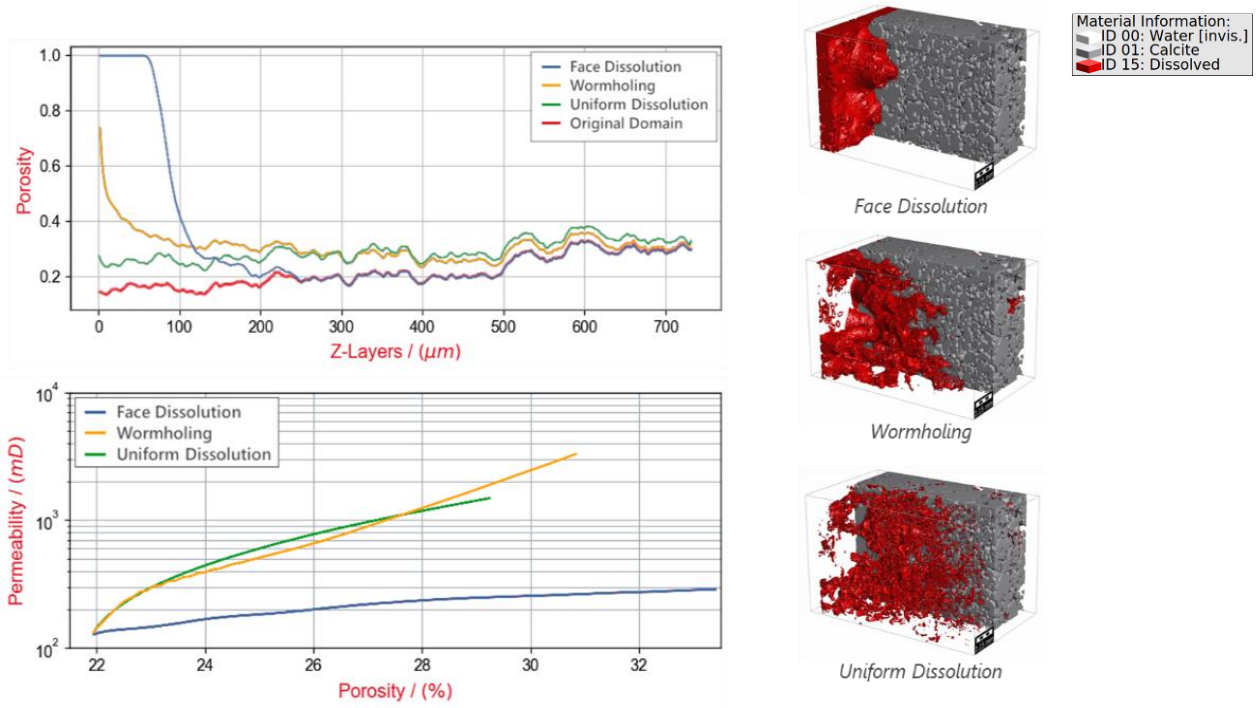


Figure 2.

Simulation of acidizing treatment in the digital Grosmont carbonate rock of Andrä et al. (2013) using different injection velocities, which results in three main different Dissolution regimes upon usage of the reaction-rate model or pH-based model to dissolve the calcite at computed particle-rock collisions.

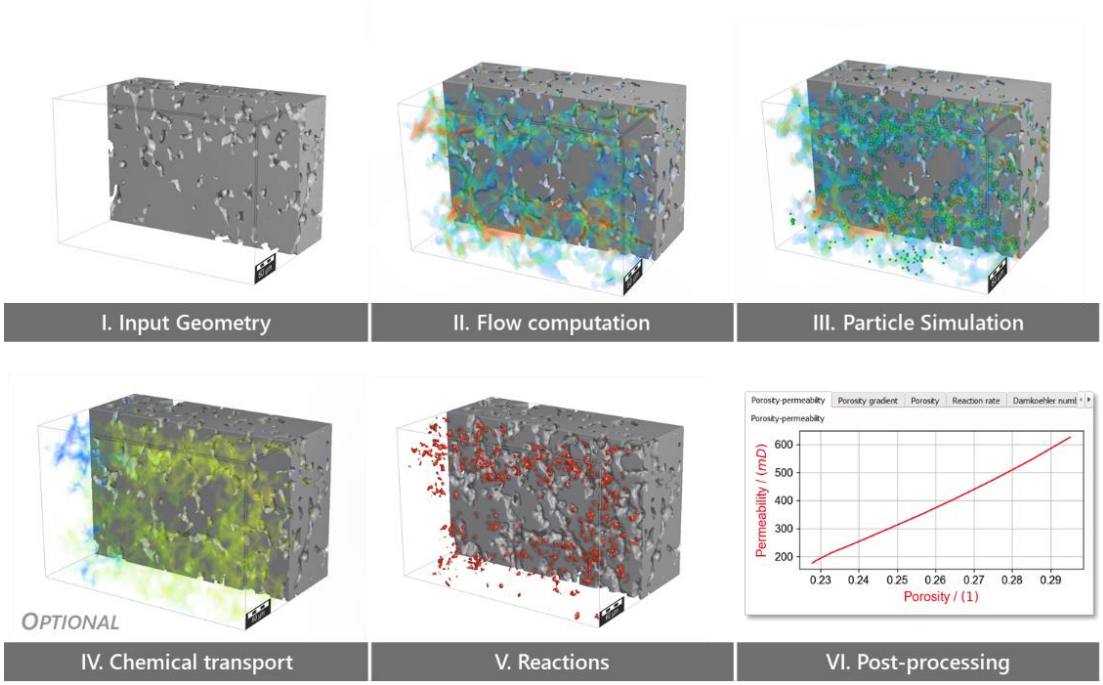


Figure 3.

The general workflow for Reactive Flow modeling in GeoDict 2021.
Step IV is only considered upon usage of the PhreeqC models.

SANDSTONE QUALITY CONTROL

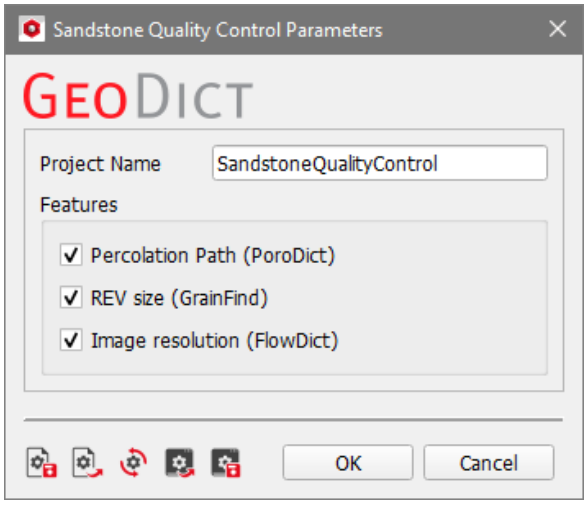
Segmented 3D digital images require a quality check. Therefore, we implemented the **Sandstone Quality Control** app to offer a user-friendly tool to perform a Quality Control specifically for segmented digital sandstone rocks based on methods and findings published by [10] and [11]. These recommendations aim at the determination of the suitability of the sample under investigation for single-phase flow computations.

Parts of the following Quality control recommendations may also be considered for other rock types and further samples.

Modules needed to run this GeoApp: PoroDict, GrainFind, and/or FlowDict

Clicking **Edit** opens the **Sandstone Quality Control Parameters** dialog.

An online workshop for this feature (amongst others) is available from here.



The usage of all the three available features is recommended (as long as the given modules are available):

- The **Percolation Path** feature investigates the pore throat resolution, which affects the computed permeability. Saxena et al. (2018) recommend a resolution of 10 voxels to sufficiently resolve pore throats for single-phase flow computations that predict the absolute permeability. For the usage of our flow solvers, we recommend a resolution of at least 4 voxels. Below 4 voxels, the runtime might increase significantly, and the permeability prediction may become inaccurate.

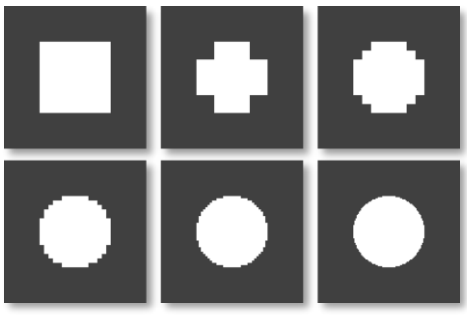


Figure 1.

Schematic representation of tubes resolved at varying voxel diameter highlighting the significant effect of the pore throat resolution on the permeability that may be predicted by numerical solvers.

- The **REV Size** considers the **R**epresentative **E**lementary **V**olume that is required to compute an absolute permeability that is representative for the rock formation under investigation. In general, an REV may be defined as a rock volume large enough that properties under investigation are insensitive to changes in rock volume and in boundary conditions of numerical tools. Saxena et al. (2018) recommend considering the ratio of the (smallest) structure length to the effective grain diameter:

$$L_{structure} > 5 * d_{Grains}$$

- The **Image Resolution** feature applies sample porosity and roughly approximated permeability (with a short computational runtime) to check if the acquired image resolution is suitable for single-phase flow computations. The applied workflow is based on findings published by [11] upon consideration of a large sandstone database.

  Curves in **Figure 2** depict the permeability that can be computed by Stokes solvers – at minimum – based on segmented porosity, image voxel size, and numerics. The permeability of the sample (red cross) should be above the numerical minimum (red cure). Otherwise, we recommend acquiring an image of higher resolution.

  If porosity and permeability are known a priori, we recommend using the additional curves as a suggestion for a suitable image resolution.

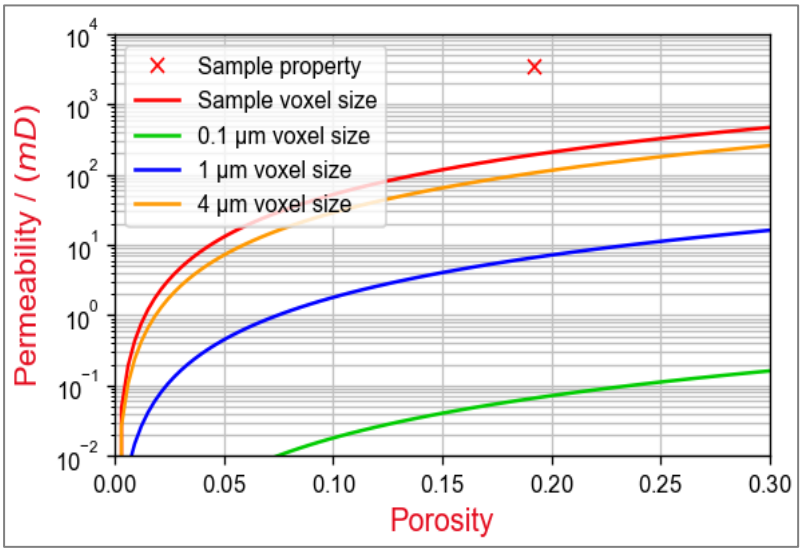


Figure 2.

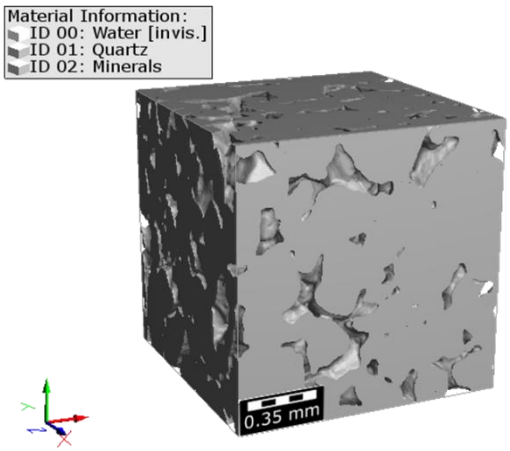
Result for a Workshop geometry (dimensions: 256³). The red curve shows the minimum permeability computable for this sample. The red cross shows a computed permeability, which is far above the numerical minimum (red curve) and thus the image resolution is fine, from this perspective.

The parameters can be modified if needed, otherwise click **OK** to close the dialog. Go back to GeoApp GUI and click **Run**.

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

The **Results → Report** tab (*below*) of the Result Viewer shows the results of the quality control.

The resolution is displayed in red in the table, but observing the plot under the **Results → Plots** tab shows, that in this case, the image resolution is fine, as explained in **Figure 2**.



Result Viewer

Tue Nov 9 2021 (2022 Build 52907) .../SandstoneQualityControl/SandstoneQualityControl.gdr

Input Map | Post Map | Results

Report | Plots | Map

Micro-CT image quality check

- The ratio N(REV) of field of view (L) and effective grain size D(eff) provides a reliable measure of REV for single-phase fluid flow in sandstones. N(REV) >= 5 is a good indicator for REV [2].
- 10 voxels are needed to sufficiently resolve pore throats for single-phase fluid flow simulations, and below 5 voxels simulations might become inaccurate [2].
- With information about porosity and permeability, recommendations for image resolution can be made. In the plot "Porosity-Permeability & Image resolution", your poro-perm value (red cross) should relatively plot above the image resolution curve (red), which depicts the minimum permeability that can be computed [1].

Average Grain Diameter	211.3 µm	
N(REV) for sandstones	6.53	For sandstones: OK for single-phase flow. (It is recommended to use the maximum available structure size for single-phase flow)
Maximum flow path diameter	**7.00 voxel**	Saxena et al. recommmend a flow path diameter of >=10 voxel, so please have a careful look at your flow results - you might need a higher resolution
Porosity	0.192	
Estimated Permeability	3418.088 mD	Please consider: This is just an estimation with low convergence settings and does not replace a suitable FlowDict computation. (Estimated permeability is in Z-direction)

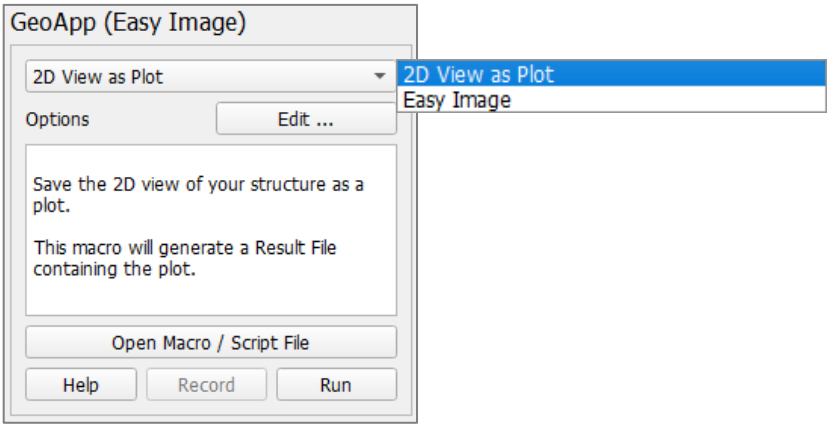
[1] Saxena, N., Hofmann, R., Alpak, F., Berg, S., Dietderich, J., Agarwal, U., Tandon, Hunter, S., Freeman, J., Ove B., References and benchmarks for pore-scale flow simulated using micro-CT images of porous media and digital rocks. Advances in Water Resources, 109, 211- 235, 2017.
[2] Saxena, N., Hows, A., Hofmann, R., Alpak, F., Freeman, J., Hunter, S., Appel, M., Imaging and computational considerations for image computed permeability: Operating envelope of Digital Rock Physics. Advances in Water Resources, 116, 127-144, 2018.

Manage Data | Load Input Map | Export | Close

EASY IMAGE

The **Easy Image** GeoApp contains the following, selectable from the pull-down menu:

- **2D View as Plot**: save the 2D view of the current structure as a plot.
- **Easy Image**: provides the possibility to create a variety of media materials, e.g., for the website, presentations, based on proofed presets**.**



2D VIEW AS PLOT

The **2D View as Plot** app saves the 2D visualization of the current structure as a plot. This plot is then contained in a GeoDict result file (*.gdr).

Modules needed to run this GeoApp: GeoDict Base

Clicking **Edit...** opens the **2D View as Plot Parameters** dialog.

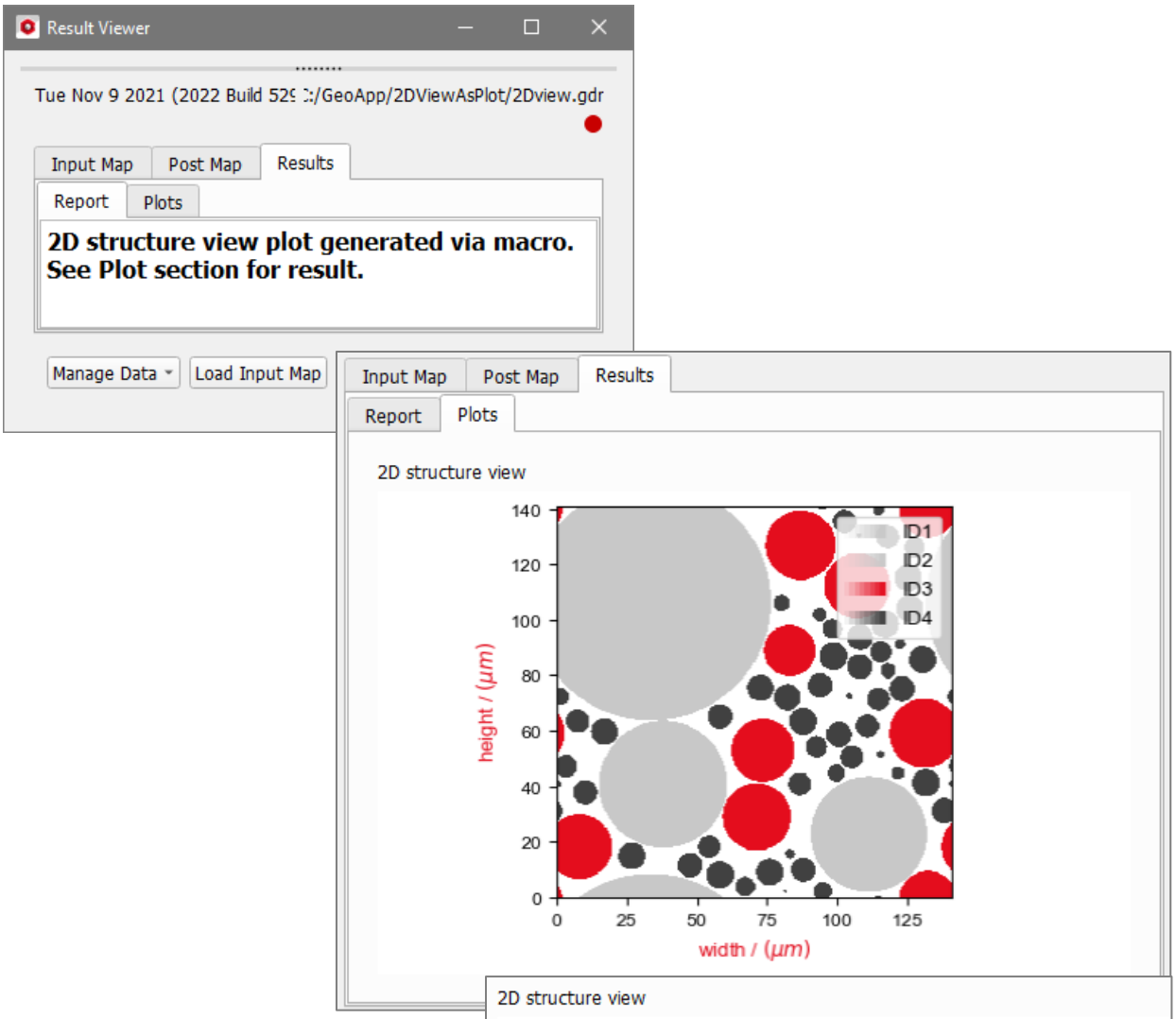
Select a **Result File Name** fitting to the current project.

Check **Use Current View** to save a plot of the currently visualized 2D slice and view direction. Otherwise select the **2D View Direction**, the **2D View Slice** and choose whether to **Show bottom to top** or not.

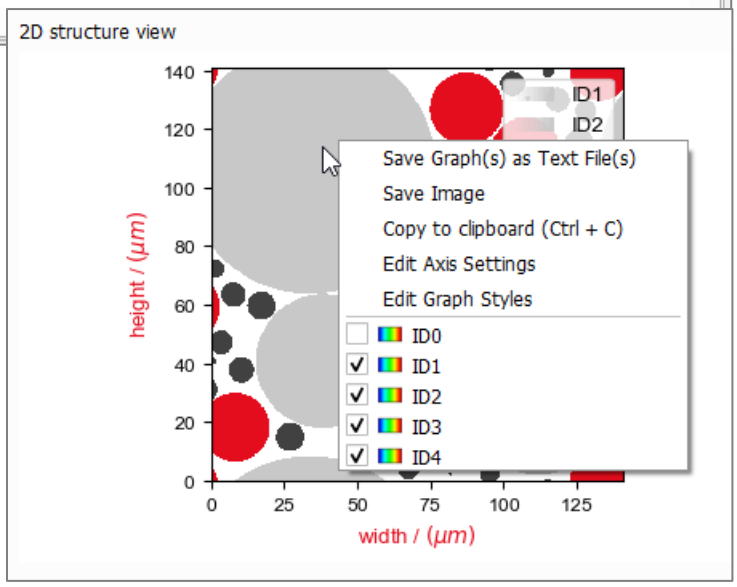
The parameters can be modified if needed. Otherwise, click **OK** to close the dialog, go back to the **GeoApp** section, and click **Run**.

When the image generation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

The **Results** → **Report** tab only displays a short report and more graphical information is found in the **Result** → **Plots** tab. There, find the resulting image from the 2D structure view.



Right-clicking in the plot opens a dialog providing several options for post-processing, as described in the Result Viewer handbook of the User Guide.



The image also is saved as *.png in the project folder.

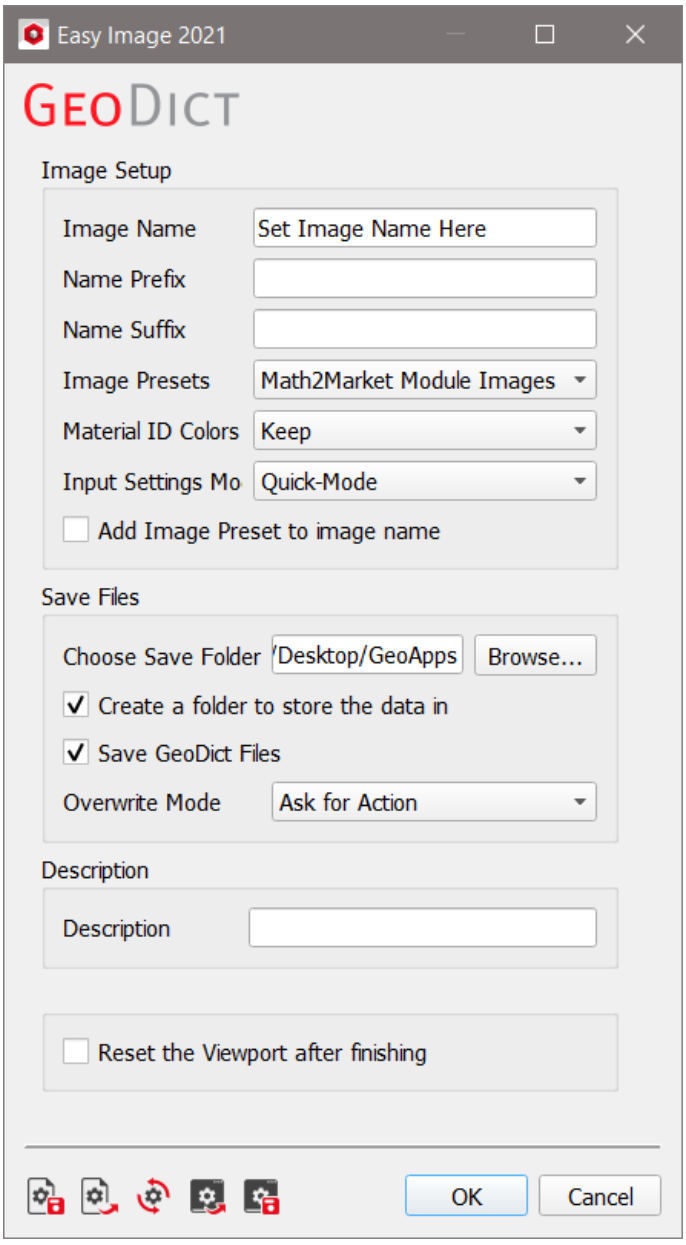
EASY IMAGE

The **Easy Image** app is designed to guide you through the steps of creating various media in an understandable way. It also saves the data needed to recreate the created media material.

Clicking **Run** opens the **3D-Image Report Parameters** dialog.

Modules needed to run this GeoApp: GeoDict Base

Here you set the basic settings, such as file naming, location and image preset selection. Tooltips describe these options in more detail.



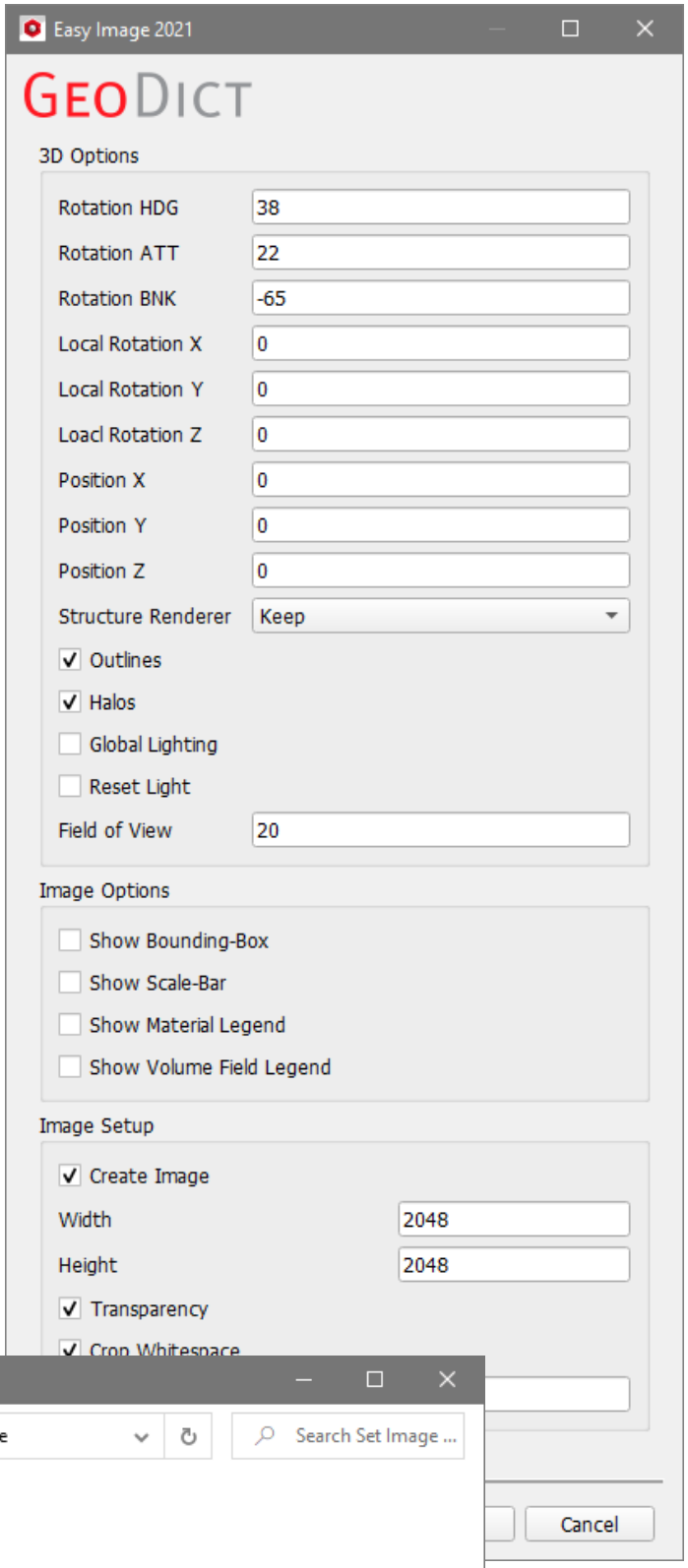
In the image presets, you can also select special modes, such as the split-by material preset. With this preset you can additionally save a video that visualizes the process of splitting.

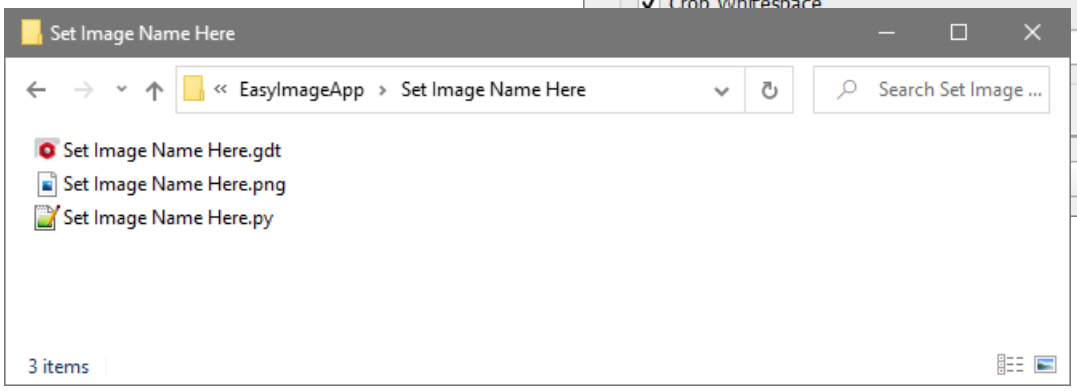
If you want to learn more about this, you can find a video tutorial here.

During image creation, additional dialogs help you to collect and save all necessary GeoDict files. Other dialogs let the user make adjustments to the image setup during image creation. On the right we see for example the Expert Mode dialog, which allows changes to the camera and visualization effects.

At the end of the image creation by the **Easy Image App**, you get a folder with the previously selected **Image Name**. **Name Prefix** and **Name Suffix** are applied only to the files stored in the folder. This way you can quickly and easily create multiple versions in the same place and not have to duplicate the necessary files.

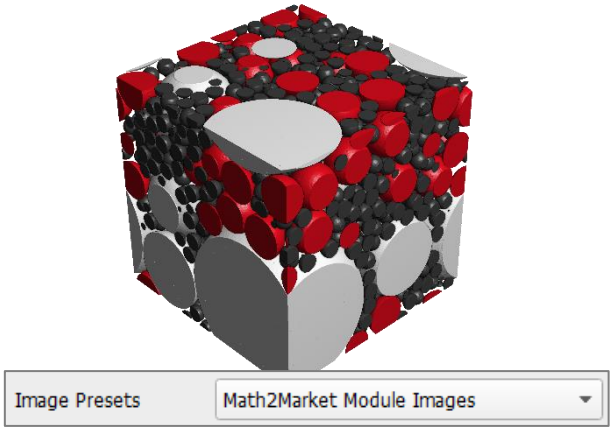
With all files in one place and the image settings saved as a Python macro, images can be reproduced quickly and easily.

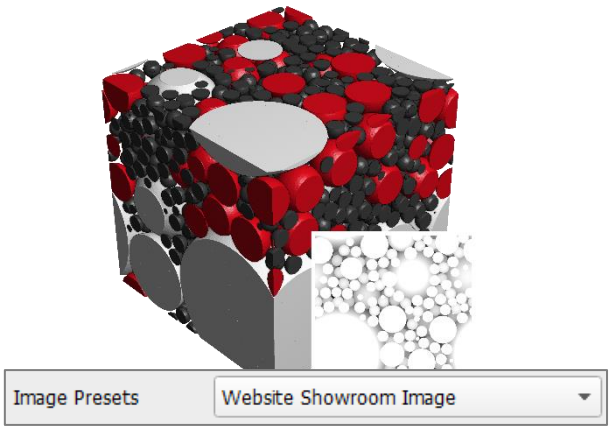


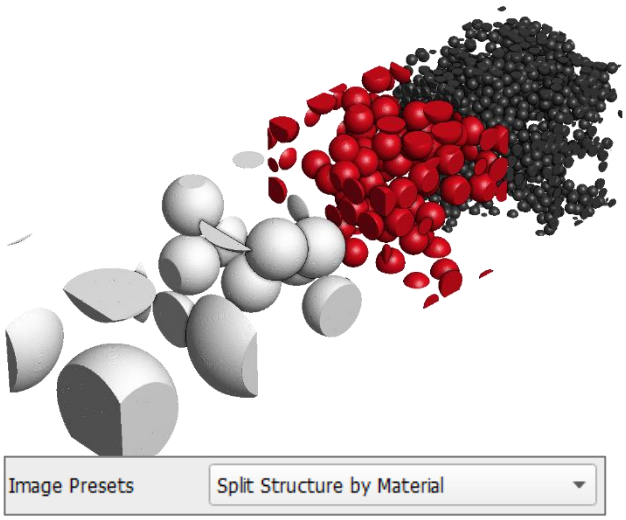


Here, three different **Image Presets** were used for the same structure, available on our website.

The **Material ID colors** were set to **GeoDict Highlight colors**. All other parameters were kept at default settings.

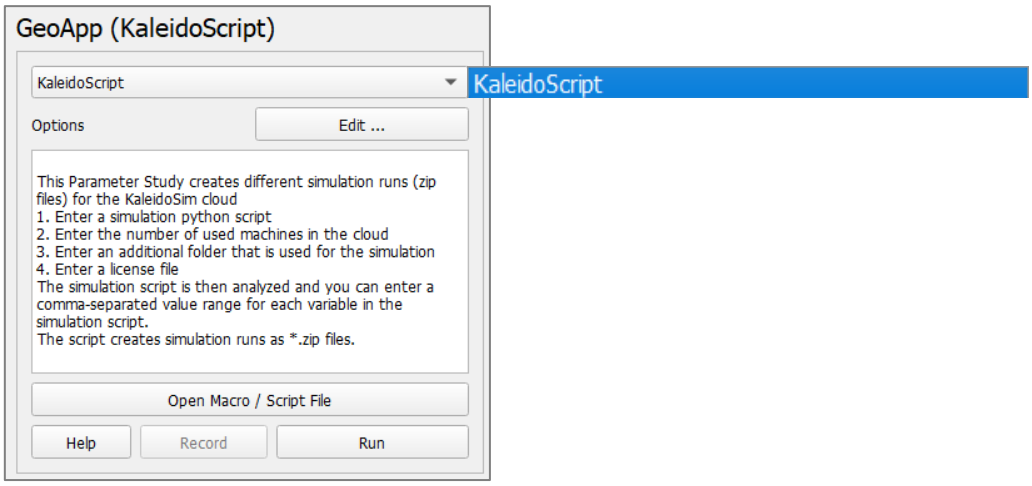






KALEIDOSCRIPT

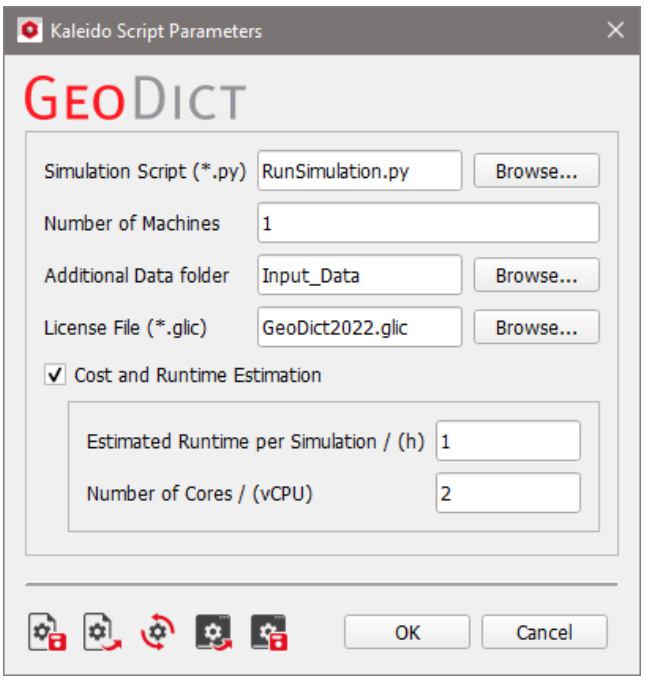
The **KaleidoScript** GeoApp helps to prepare all needed files for a GeoDict run in the KaleidoSim cloud. If the available hardware does not allow to run GeoDict simulations on big structures or at least not in time, clouds offer efficient solutions. For the KaleidoSim cloud a GeoPy macro must be recorded in GeoDict. Learn the details of macro recording and editing in the Automation & Scripting User Guide. Simply record a macro of the desired GeoDict commands and open the macro in a text editor, e.g. Notepad++, to add the needed variables.



Modules needed to run this GeoApp:GeoDict-Base

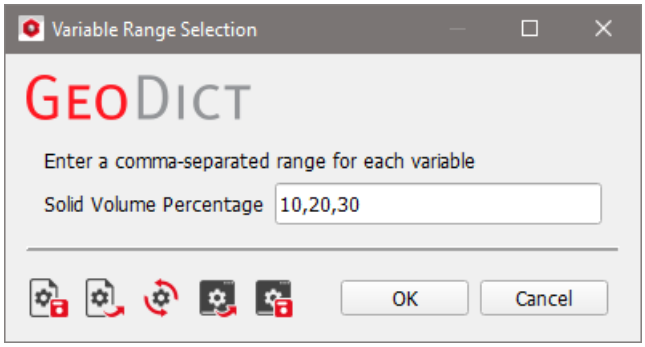
Clicking **Edit** opens the **KaleidoScript Parameters** dialog.

- Browse for a **Simulation Script (*.py)** recorded in GeoDict.
- Select the **Number of Machines** used in the KaleidoSim cloud.
- Select an **Additional Data Folder.**
- Browse for the GeoDict **License File (*.glic)** created for KaleidoSim. Apply for a KaleidoSim license on licenses@math2market.de.
- Select **Cost and Runtime Estimation** to obtain an estimation of total costs and the runtime on the KaleidoSim cloud based on the entered **Estimated Runtime per Simulation** and **Number of Cores**.

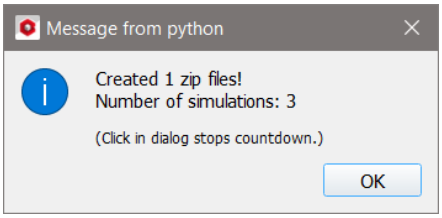


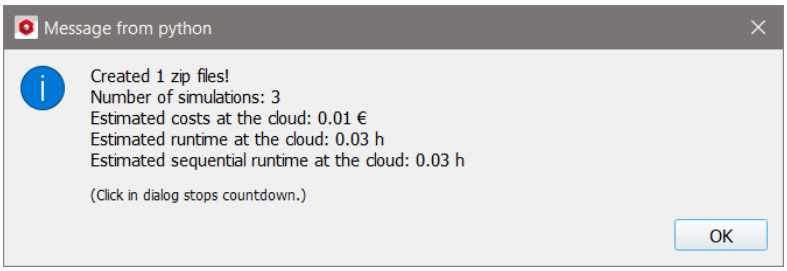
Click **OK** to close the parameters dialog and **Run** to start the **KaleidoScript** app.

A dialog appears to enter comma-separated value lists for each variable in the selected simulation script. Here, only the Solid Volume Percentage of the generated structure.

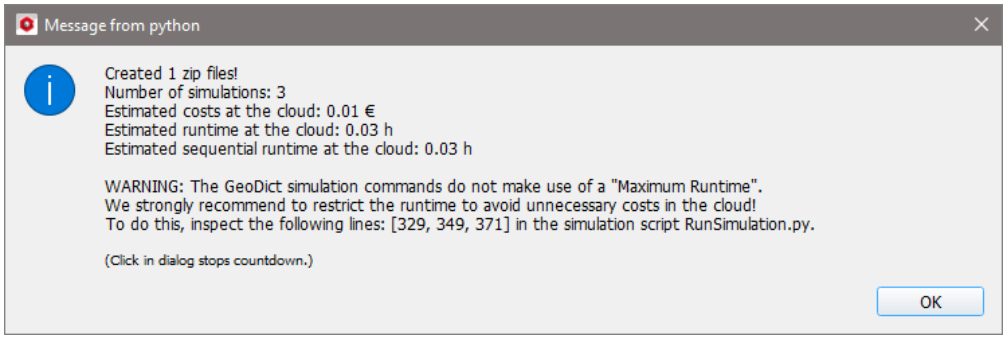


After entering the desired value lists click **OK**. Finally, a message dialog shows the results of the **KaleidoScript**. If **Cost and Runtime Estimation** was selected, also the estimated costs and runtime can be found in the message dialog.

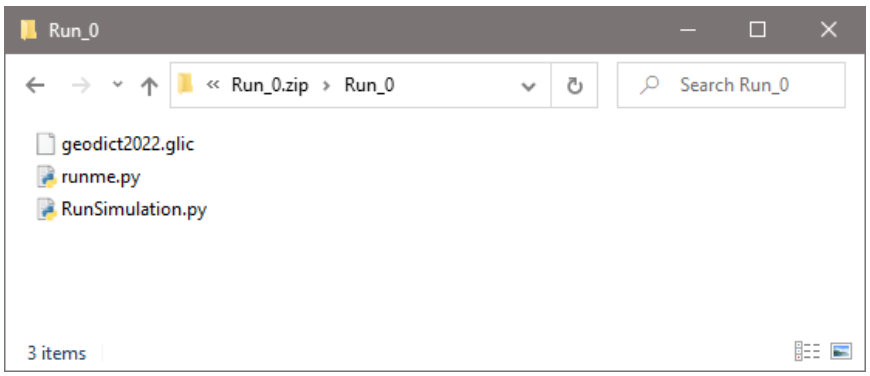




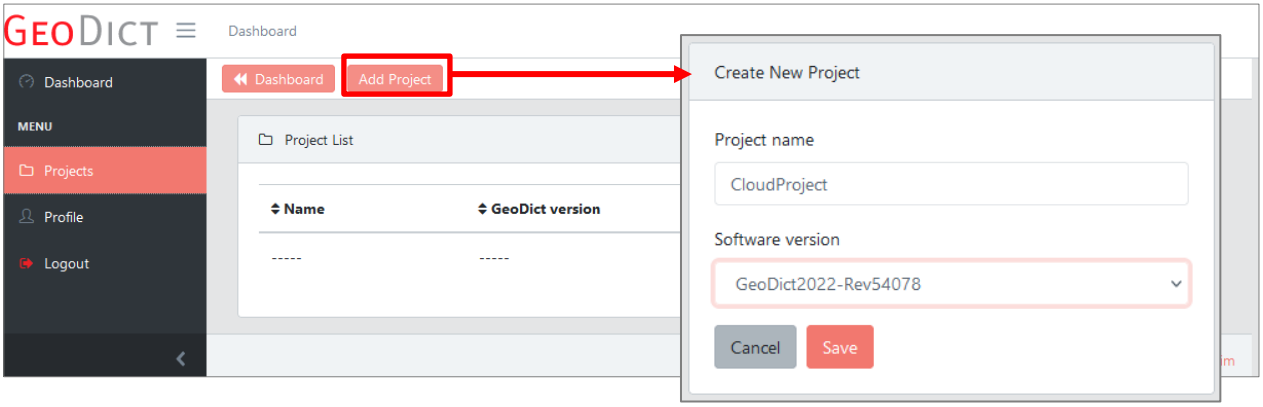
If the **Maximum Runtime** was not specified in the **Simulation Script**, a warning recommends restricting the runtime to avoid unnecessary costs in the cloud.



In the **Project Folder** find a *.zip folder for each parameter combination. In this case, the simulation script had one variable and three values were entered. Thus, the folders **Run_0.zip, Run_1.zip**, and **Run_2.zip** are created, each containing the GeoDict license **geodict2022.glic** for the KaleidoSim cloud, the GeoPy script **runme.py**, containing the corresponding value for the simulation script, and the simulation script itself.

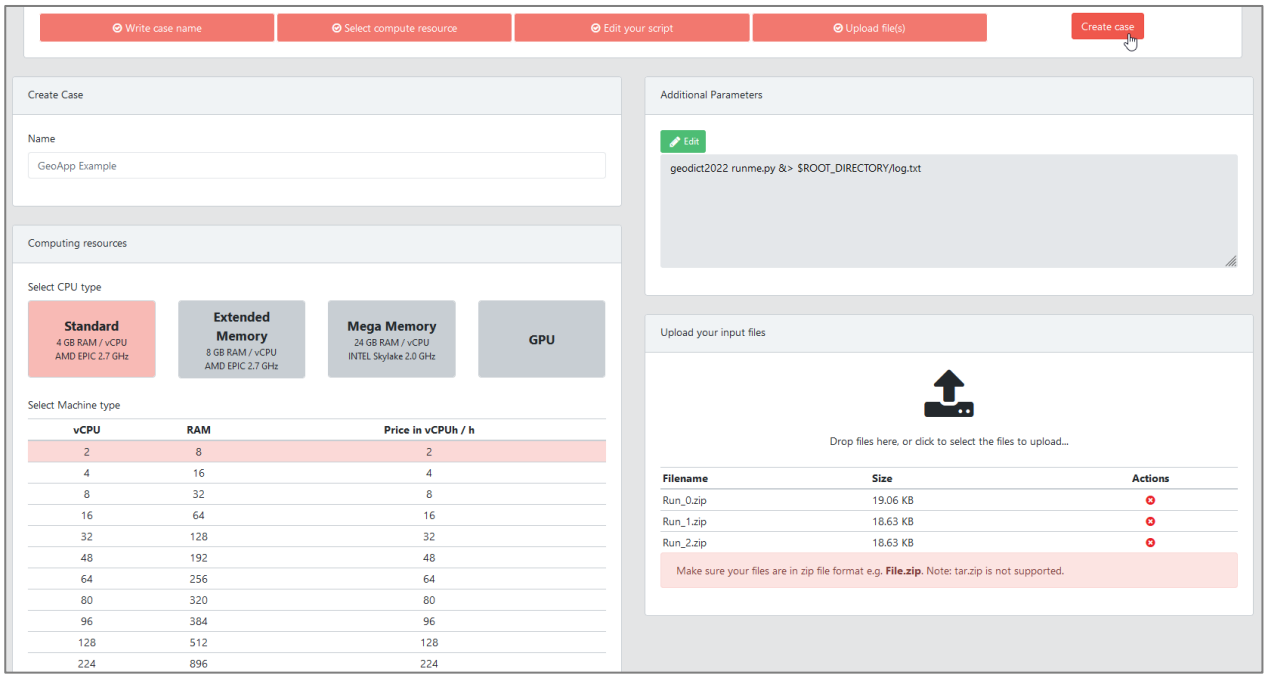


To run the simulation in the KaleidoSim cloud log in. Then, under the **Projects** tab select **Add Project**, enter a **Project name** and select a **Software version** from the pull-down menu. Click **Save** and a new project is opened.

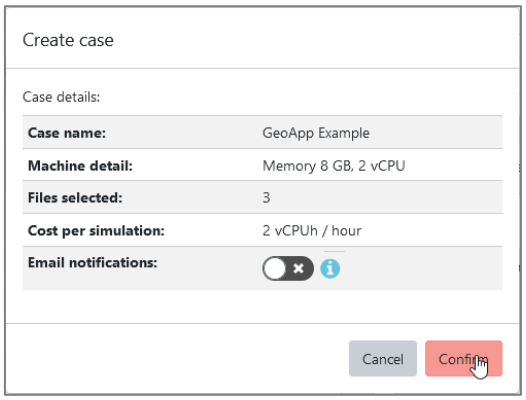


Next, click **Create case.**

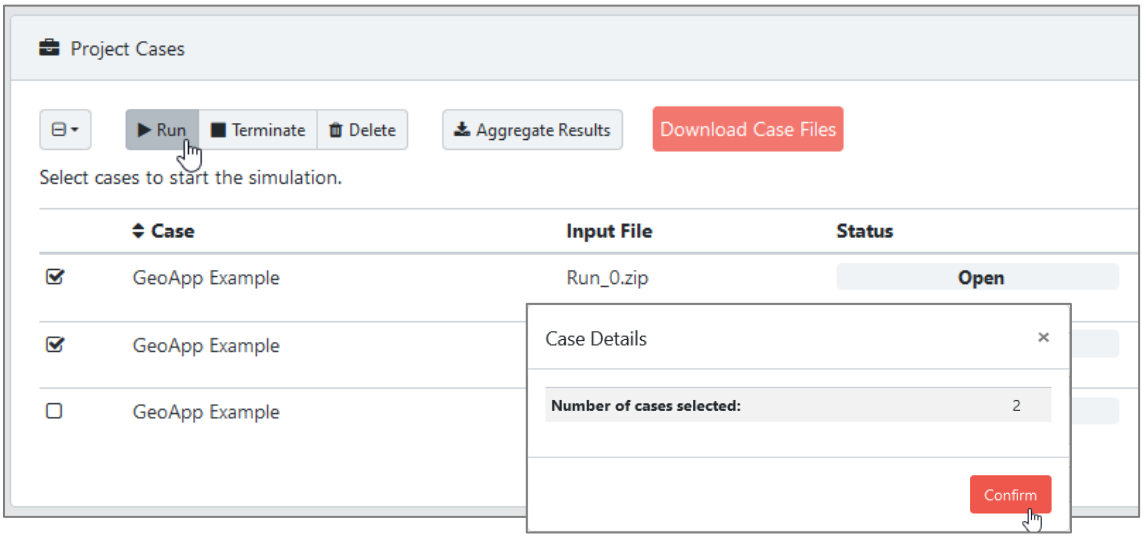
Enter a **Name**, select a machine type and upload the zip files created by the **KaleidoScript** app. Additionally the command line parameters can be adjusted, if needed.



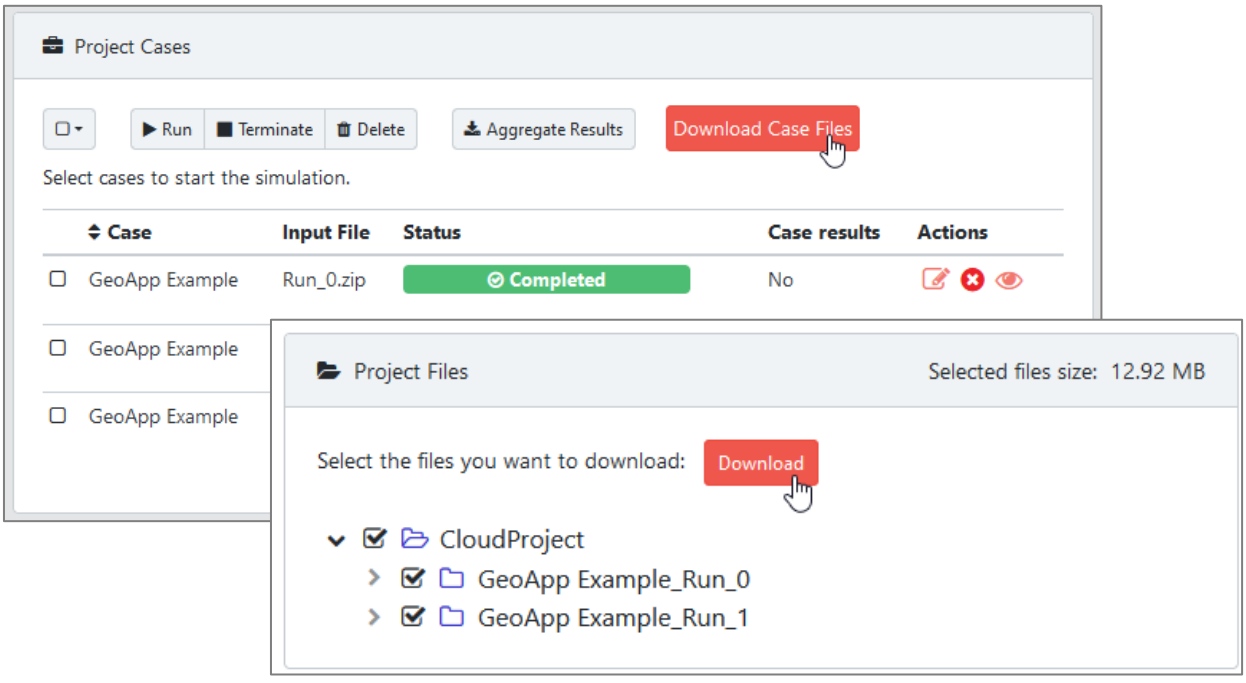
Click **Create Case** and **Confirm** the case details.



In the **Project Cases** panel select the desired runs of the case and click **Run** and **Confirm**.



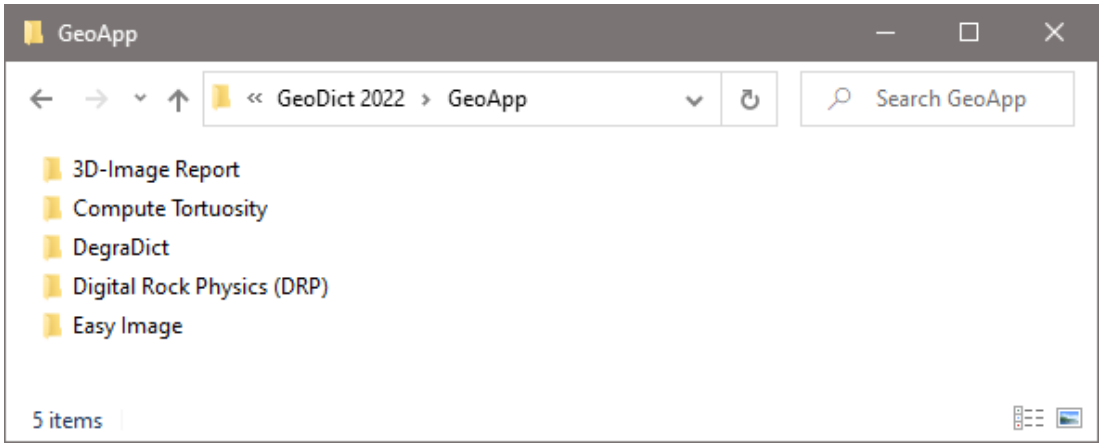
When the simulations are finished, the **Status** is set to **Completed** and the results can be downloaded by clicking **Download Case Files**, selecting the files to download and clicking **Download**.



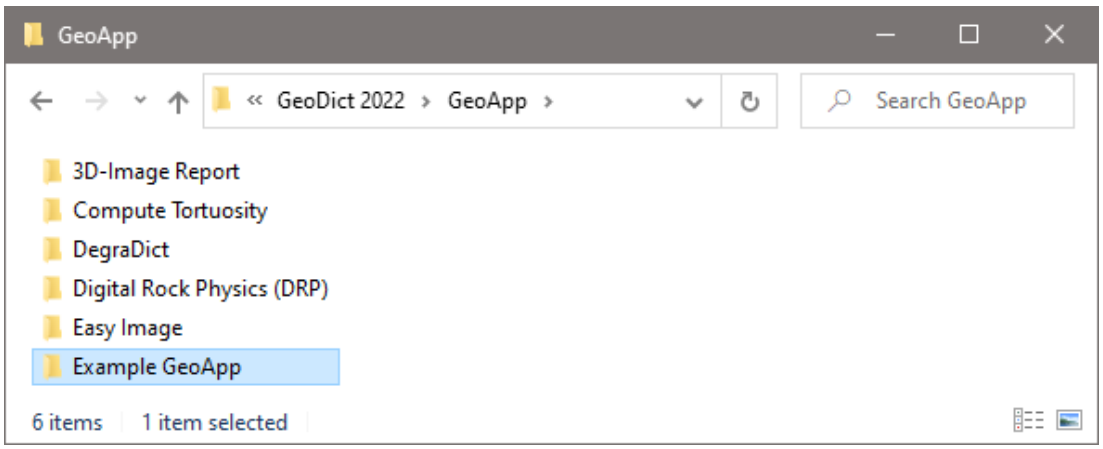
ADDING CUSTOM GEOAPPS

The GeoApps are stored in the **GeoApp** folder included in the GeoDict installation folder. The **Module Predefined** apps are located in the corresponding module folders e.g., the GeoApps for FiberGeo are to be found in the **FiberGeo** folder in the GeoDict installation folder.

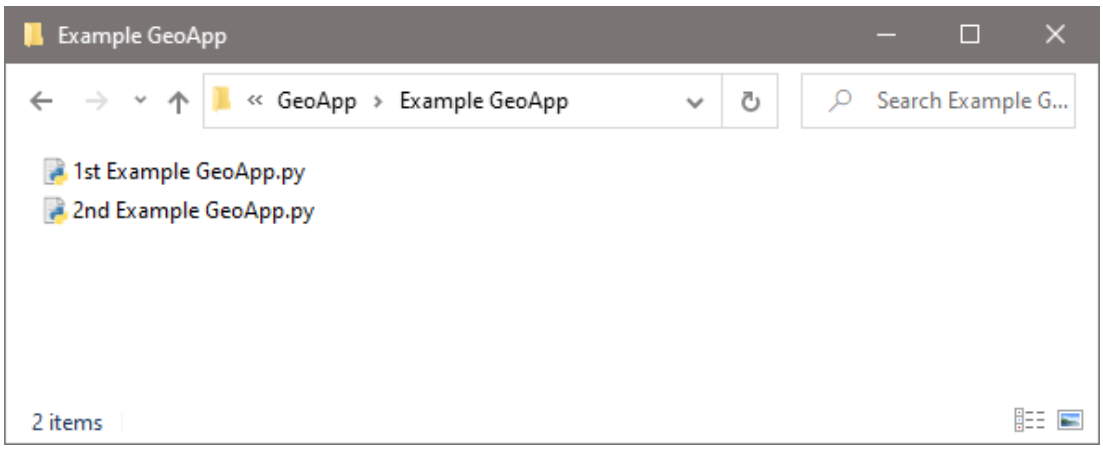
Below, the apps that are located in the folder **C:\Program Files\Math2Market GmbH\GeoDict 2022\GeoApp** are shown. Five **GeoApps** are included in the standard installation package, but additional apps may be placed there by the system administrator and would then be available for all users.



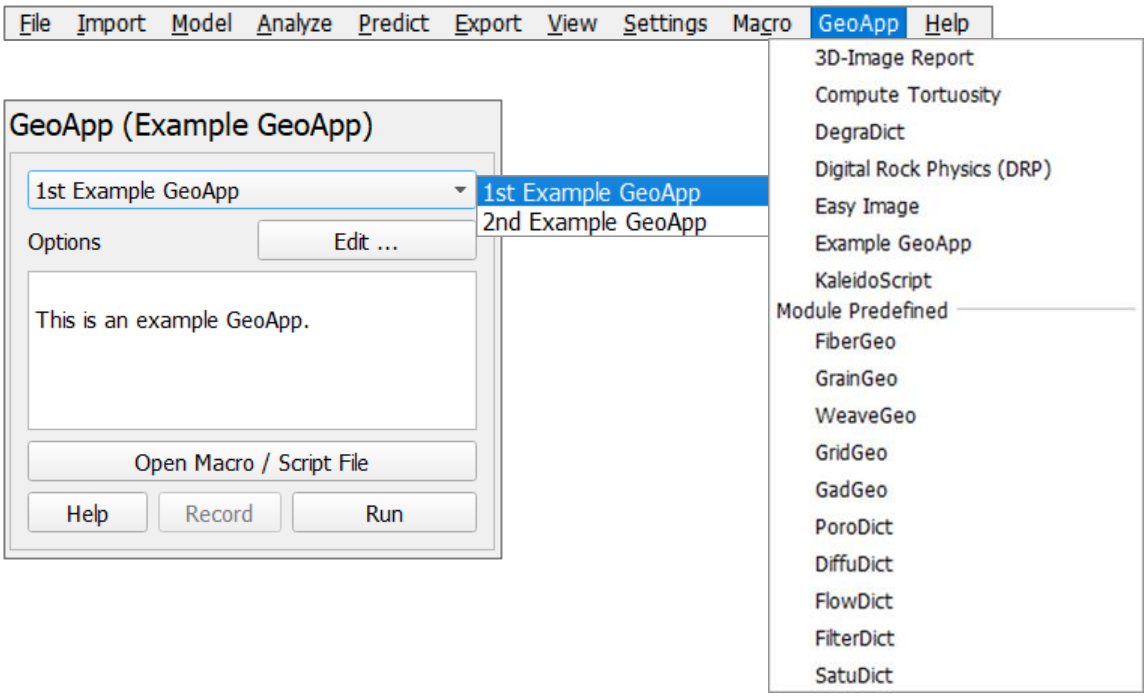
Therefore, create a new folder inside the **GeoApp** folder. In the example below, the **Example GeoApp** folder is added. The name of this folder will be displayed later under the GeoApp menu in the GeoDict Graphical User Interface (GUI).



In the new folder, place the GeoPy files that will be selectable from the pull-down menu in the new GeoApp. Here, for example, the two scripts: **1st Example GeoApp.py** and **2nd Example GeoApp.py.** How to create a GeoPy file containing parameters accessible from the GeoDict GUI is described in the Automation by Scripting handbook of this User Guide.



After restarting GeoDict, the new app will be available from the GeoApp menu. If selected, in the GeoApp section the new apps are displayed and can be edited and run as described on pages 1ff.



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